Supporting Information

Synthesis of pyrrolo[1,2-*a*]quinoxalines via electrochemical C(sp^3)-H functionalization

Sijie Peng[a], Tong Li[a], Kai Li[a], Qi Sun[*b] and Zhiyong Wang[*a,b]

*Hefei National Center for Physical Sciences at Microscale, Key Laboratory of Precision and Intelligent Chemistry, School of Chemistry and Materials Science, University of Science and Technology of China, Hefei 230026, China.
*E-mail: zwang3@ustc.edu.cn
*Institute of Advanced Technology, University of Science and Technology of China. Hefei 230000, China.
*Email: sunqi924@ustc.edu.cn

Table of Contents

General Information S2
Experimental Procedure S2
Optimization of Reaction Conditions.....S7
Cyclic Voltammetry Data S8
Detail Descriptions for Products S10
References S18
Copies of Product NMR Spectra S18

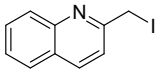
General Information

Unless otherwise noted, materials were obtained from commercial suppliers and used without further purification. NMR spectra were recorded on a Bruker AV-500 (^{1}H: 500 MHz, ^{13}C: 125 MHz, ^{19}F: 470 MHz) spectrometer using TMS as internal reference. Chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz, respectively. The following calibration was used: $CDCl_3$ δ = 7.26 and 77.16 ppm, THF δ = 1.72, 3.58 ppm and 67.21, 25.31 ppm. GCMS was Shimadzu QP-5050 GC-MS system. Commercially available compounds were used without further purification. All substances were known compounds and synthesized according to the literature. High resolution mass spectra (HRMS) were measured using electrospray ionization (ESI) and the time-of-flight (TOF) mass analyzer. The anode electrode and cathode electrode all are Pt (1.0 × 1.0 cm^2). These electrodes are commercially available from GaossUnion, China.

Experimental Procedure

Procedure for the preparation of 4 (2-(iodomethyl)quinoline):

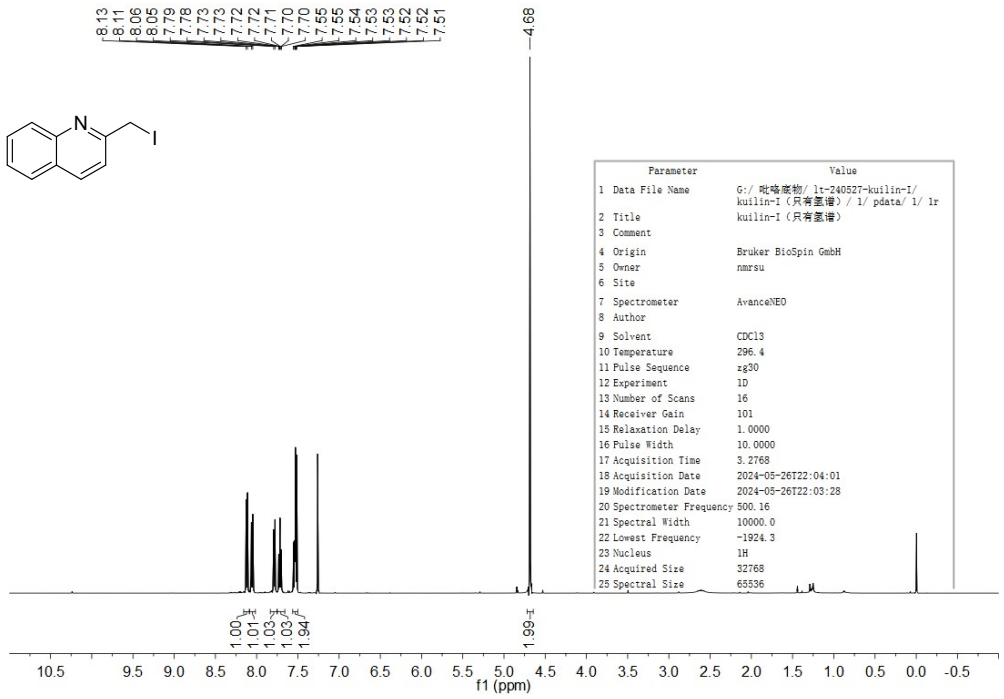
2-Methylquinoline (**1a**, 0.5 mmol), cuprous halide (0.75 mmol), TBHP (8.0 eq., 70% aqueous solution) and CH_3CN (2 mL) were stirred at 70 °C for 8 h. Then, the reaction mixture was diluted by water and extracted with CH_2Cl_2 (3×15 mL). The I_2 in organic phase was quenched by $Na_2S_2O_3$. The combined organic layers were washed with saturated NH_4Cl aqueous solution and dried over anhydrous Na_2SO_4. After filtration, the solvent was evaporated in vacuo. The desired product was obtained by silica gel chromatography (petroleum ether/ethyl acetate, v/v=10/1).[S1]



2-(iodomethyl)quinoline

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 1H), 8.06 (d, *J* = 8.5 Hz, 1H), 7.79 (d, *J* = 8.1 Hz, 1H), 7.73-7.69 (m, 1H), 7.57-7.49 (m, 2H), 4.68 (s, 2H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.4, 147.5, 137.3, 130.0, 129.0, 127.5, 127.1, 126.9, 121.1, 6.8.



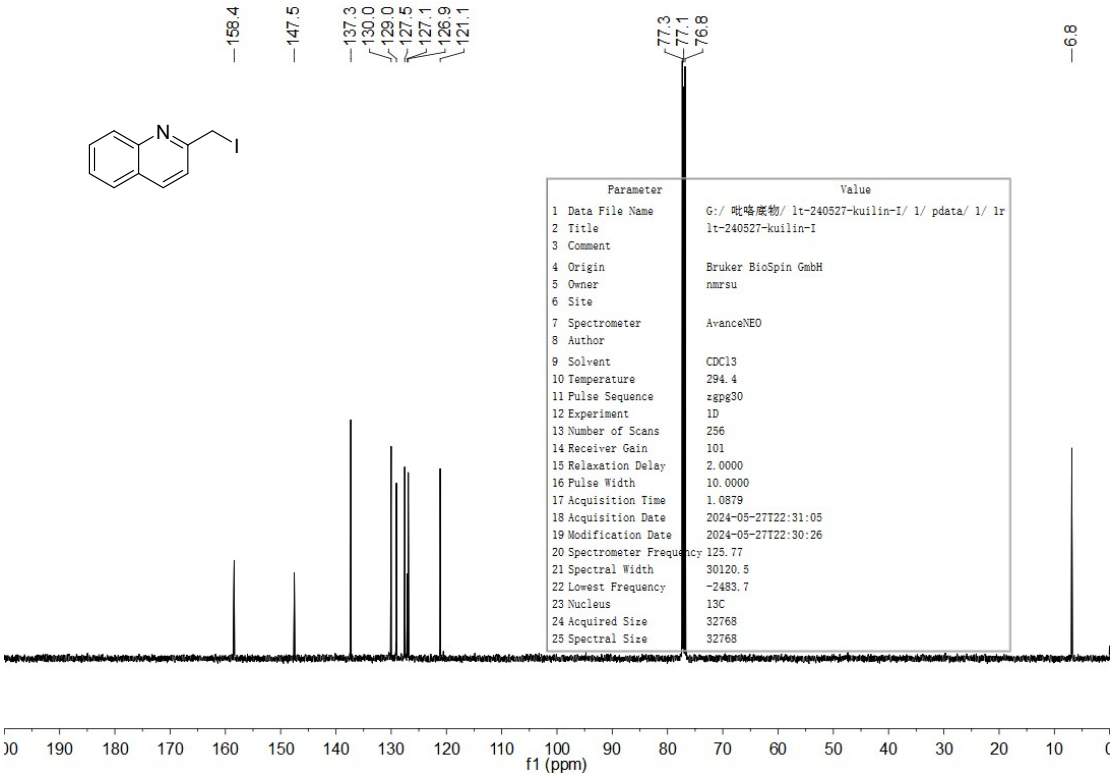


Fig S1. The NMR spectra of the prepared 2-(iodomethyl)quinoline

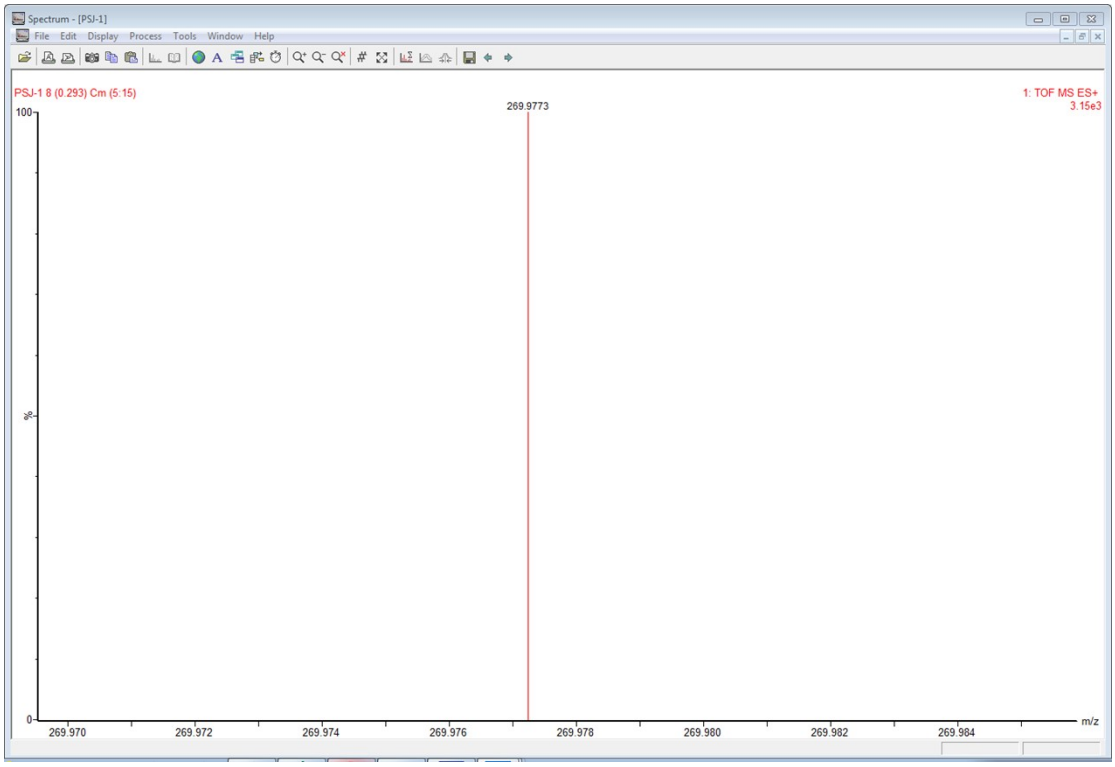
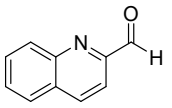


Fig. S2 The HRMS data of intermediate **4** detected during the reaction process

Procedure for the preparation of 5 (quinoline-2-carbaldehyde):

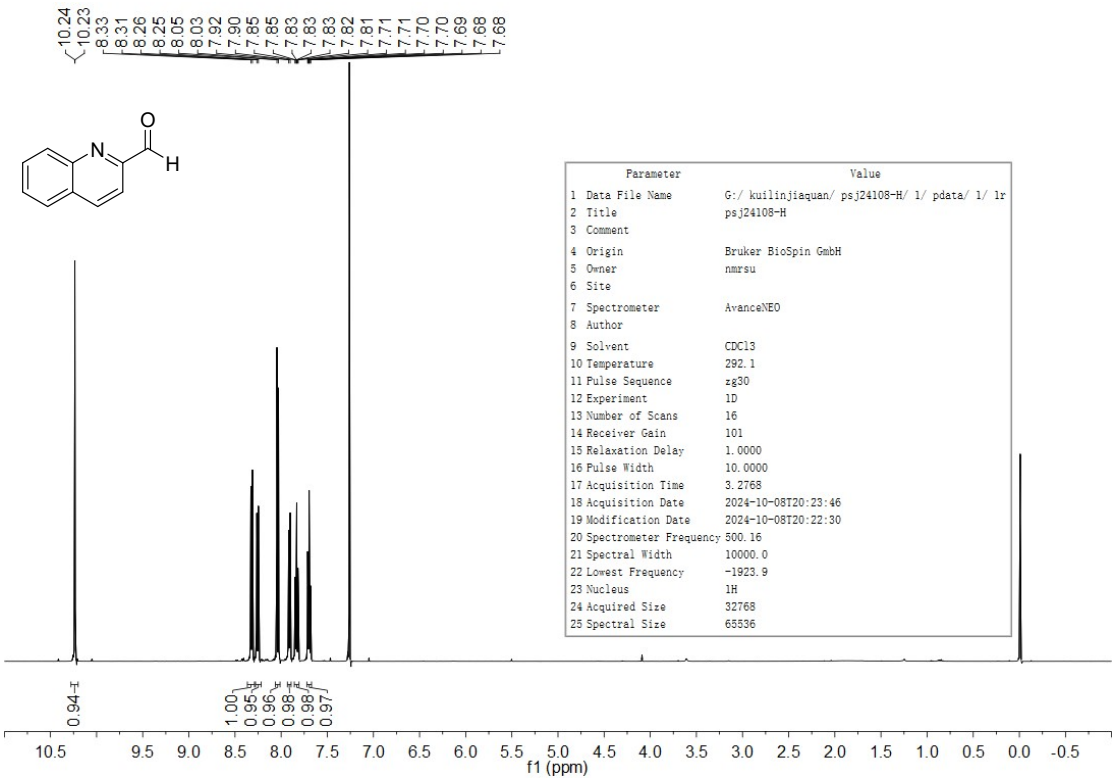
A 25 mL pressure vial was charged with 2-methylquinoline (43.0 mg, 0.30 mmol, 1.0 equiv.), I_2 (7.6 mg, 0.03 mmol, 0.1 equiv.), TFA (68.4 mg, 0.6 mmol, 2.0 equiv.) and DMSO (2.0 mL). The vial was sealed and the resulting mixture was stirred at 130 °C for 30 min under an air atmosphere. After the reaction was completed (monitored by TLC), and added 50 mL water and an appropriate amount of 10% NaOH solution (w/w) to the mixture, then extracted with EtOAc 3 times (3 × 50 mL). The extract was washed with 10% $Na_2S_2O_3$ solution (w/w), dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel to yield the corresponding product as a brown solid (30 mg, 64% yield). [S2]



quinoline-2-carbaldehyde

^{1}H NMR (500 MHz, $CDCl_3$) δ 10.23 (d, *J* = 0.6 Hz, 1H), 8.32 (d, *J* = 8.4 Hz, 1H), 8.25 (d, *J* = 8.5 Hz, 1H), 8.04 (d, *J* = 8.4 Hz, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.86 – 7.81 (m, 1H), 7.72 – 7.67 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 193.8, 152.6, 147.9, 137.5, 130.6, 130.4, 130.1, 129.3, 127.9, 117.4.



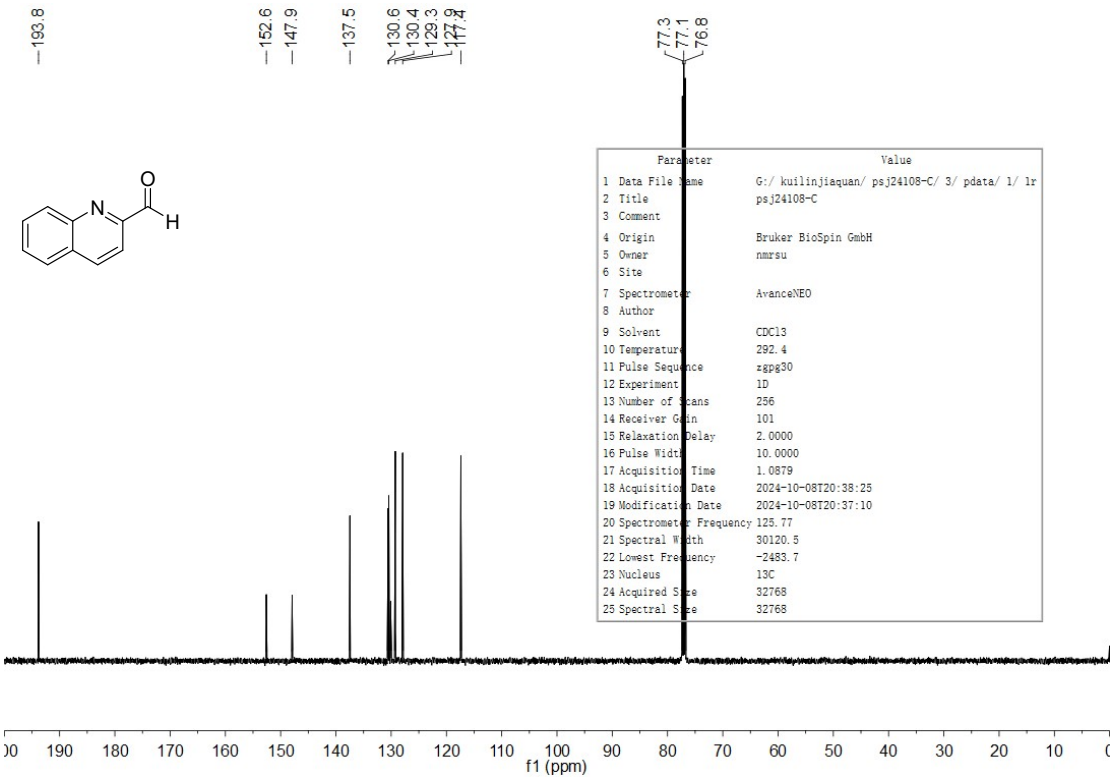
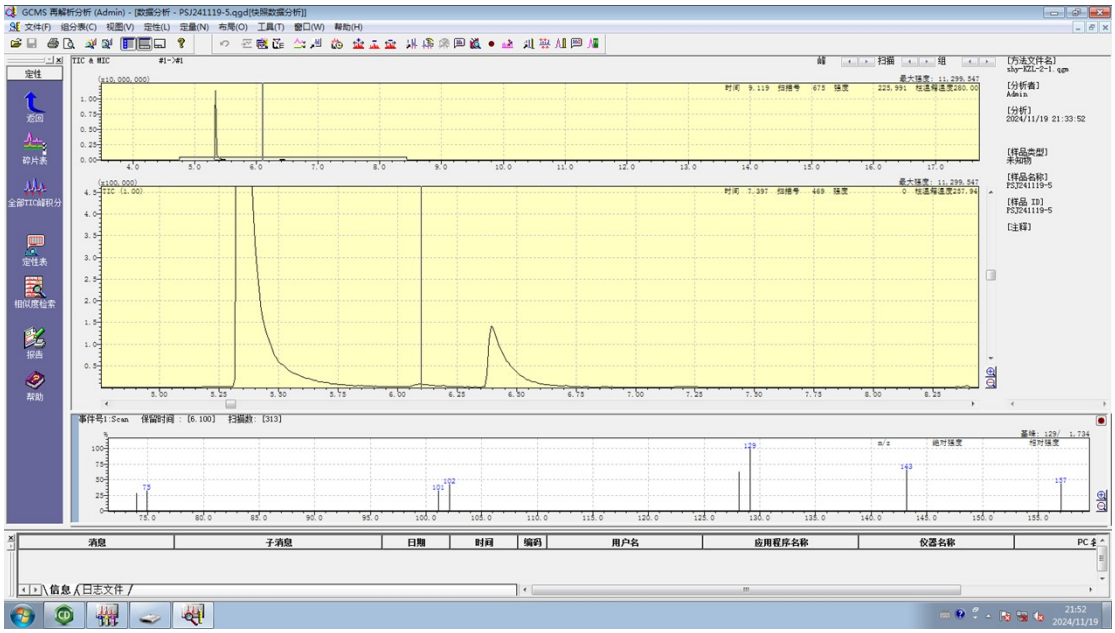


Fig. S3 The NMR spectra of the prepared quinoline-2-carbaldehyde



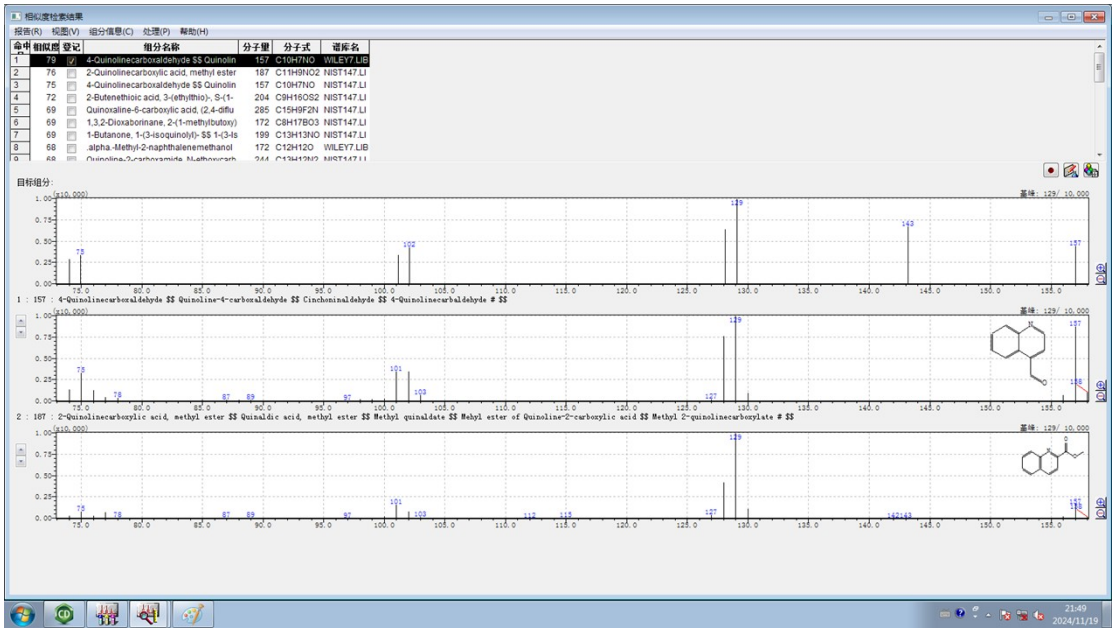


Fig. S4 The GC-MS data of intermediate **5** detected during the reaction process

Typical Procedure for the Electrosynthesis of pyrrolo[1,2-*a*]quinoxalines N-heterocycles:

A mixture of 2-methylquinoline **1a** (0.36 mmol) and 2-(1*H*-pyrrol-1-yl)aniline **2a** (0.9 mmol), $H_2C_2O_4$ (0.3 mmol), NH_4Cl (0.3 mmol) and NH_4I (0.06 mmol) and DMSO = 3 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed at a constant current of 10 mA under 100 ℃ for corresponding time. When the reaction was finished, the solution was extracted with EtOAc (3×10 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 10:1) to afford the desired product.

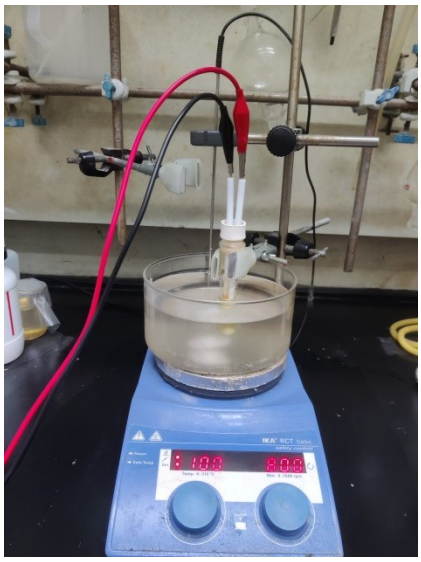


Fig. S5 The reaction setup for the electrochemical reaction

Gram-scale synthesis of 3aa:

A mixture of 2-methylquinoline **1a** (6 mmol), 2-(1*H-pyrrol*-1-yl)aniline **2a** (5 mmol), $H_2C_2O_4$ (5 mmol), NH_4Cl (5 mmol) and NH_4I (1 mmol) and DMSO = 50 mL was added to an undivided cell. The cell was equipped with platinum electrode as both the anode and cathode. The reaction mixture was stirred and electrolyzed (J = 10 mA/cm^2 , I = 23 mA) under 100 ℃ for 3.5 days. When the reaction was finished, the solution was extracted with EtOAc (3×100 mL). The combined organic layer was dried with Na_2SO_4, filtered. The solvent was removed with a rotary evaporator. The residue was purified by column chromatography on silica gel (PE/EtOAc = 10:1) to afford the desired product.

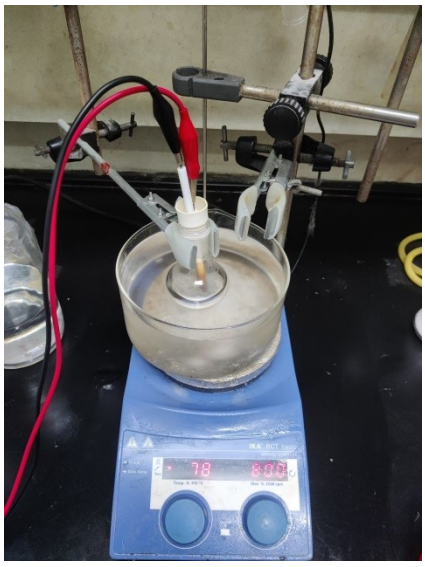
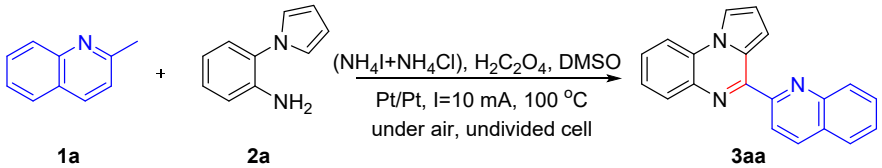


Fig. S6 The reaction setup for the gram-scale reaction

Fig. S7 Pt electrode used in the gram-scale reaction

Table S1. Optimization of reaction conditions



1a **2a** **3aa**

Entry	Variations from standard conditions	Yield[%]
1	None	81
2	DMF as the solvent	55
3	NMP as the solvent	Trace
4	Bu_4NI as the electrolyte instead of NH_4I	36

5	KI as the electrolyte instead of NH_4I	Trace
6	a graphite plate as cathode	64
7	a graphite plate as anode	Trace
8	7 mA, 15 mA instead of 10 mA	60, trace
9	90 ℃, 110 ℃ instead of 100 ℃	30, trace
10	NH_4Br, $(NH_4)_6Mo_7O_{24}·4H_2O$ instead of NH_4Cl	69, 80
11	without electricity	Trace

[a] Standard conditions 1: platinum plate (10 mm × 10 mm × 0.2 mm) as the anode, platinum plate (10 mm × 10 mm × 0.2mm) as the cathode, undivided cell, **1a** (0.36 mmol), **2a** (0.3 mmol), $H_2C_2O_4$ (0.3 mmol), NH_4I (0.06 mmol), NH_4Cl (0.3 mmol) and DMSO (3 mL), Air, 100 ℃, 12 h.

[b] The isolated yields after column chromatography.

Cyclic Voltammetry Data

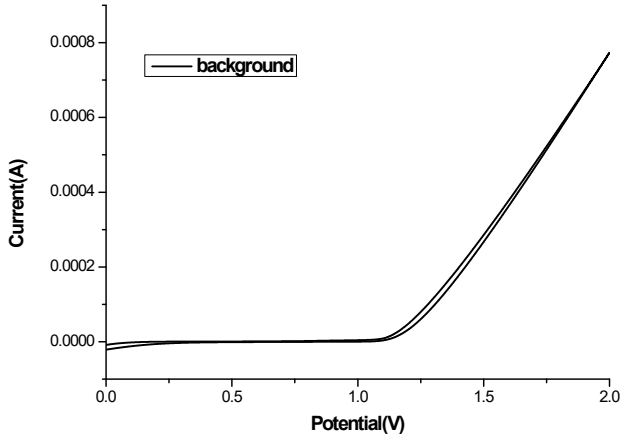


Fig. S8 Cyclic voltammetry experiments. Cyclic voltammograms of **1a**, **2a,** NH_4I and **4** in 0.1 M NH_4Cl/DMSO using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, respectively, at a scan rate of 100 mV/s: background.

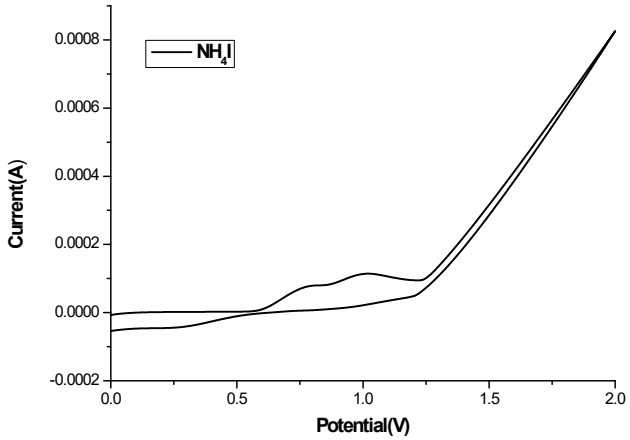


Fig. S9 Cyclic voltammetry experiments. Cyclic voltammograms of **1a**, **2a,** NH_4I and **4** in 0.1 M NH_4Cl/DMSO using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, respectively, at a scan rate of 100 mV/s: NH_4I (2 mmol/L).

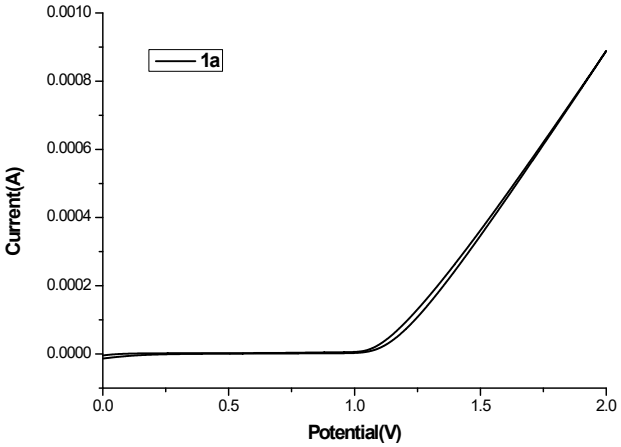


Fig. S10 Cyclic voltammetry experiments. Cyclic voltammograms of **1a**, **2a,** NH_4I and **4** in 0.1 M NH_4Cl/DMSO using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, respectively, at a scan rate of 100 mV/s: **1a** (5 mmol/L).

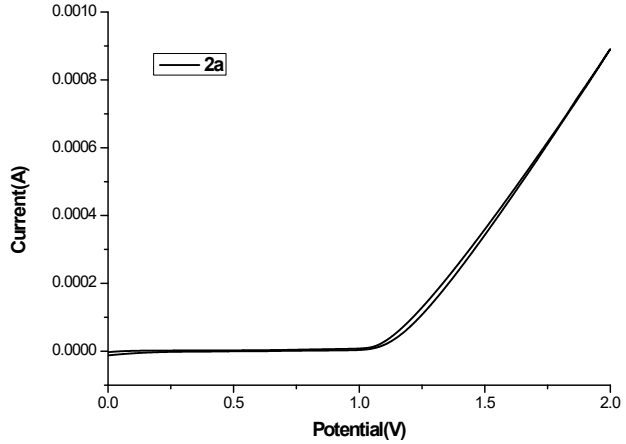


Fig. S11 Cyclic voltammetry experiments. Cyclic voltammograms of **1a**, **2a,** NH_4I and **4** in 0.1 M NH_4Cl/DMSO using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes, respectively, at a scan rate of 100 mV/s: **2a** (5 mmol/L).

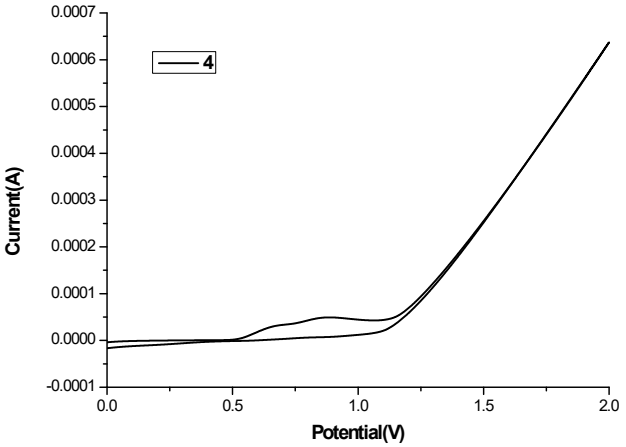
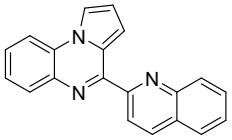


Fig. S12 Cyclic voltammetry experiments. Cyclic voltammograms of **1a**, **2a,** NH_4I and **4** in 0.1 M NH_4Cl/DMSO using a Pt disk as the working electrode, and Pt wire and Ag/AgCl as the counter and reference electrodes,

respectively, at a scan rate of 100 mV/s: **4** (5 mmol/L).

Detail descriptions for products

4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3aa)[S3]

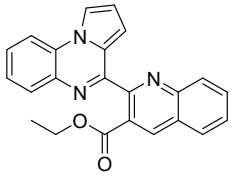


The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 81% yield, 71.8 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.65 (d, *J* = 8.6 Hz, 1H), 8.31 (dd, *J* = 11.8, 8.6 Hz, 2H), 8.18 – 8.10 (m, 2H), 8.08 – 7.99 (m, 1H), 7.90 (dd, *J* = 7.7, 4.8 Hz, 2H), 7.83-7.76 (m, 1H), 7.61 (t, *J* = 7.5 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.52-7.45 (m, 1H), 7.06 – 6.97 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.1, 150.9, 147.6, 136.4, 135.6, 130.5, 130.1, 129.6, 128.3, 128.3, 127.8, 127.6, 127.3, 125.2, 124.7, 120.7, 114.7, 114.4, 113.7, 111.4.

ethyl 2-(pyrrolo[1,2-*a*]quinoxalin-4-yl)quinoline-3-carboxylate(3ba)



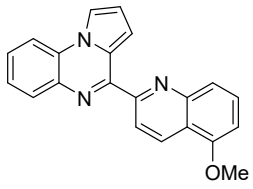
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 65% yield, 71.6 mg. m.p. 120-122 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.80 (s, 1H), 8.26 (d, *J* = 8.5 Hz, 1H), 7.79-8.04 (m, 3H), 7.92 (d, *J* = 8.2 Hz, 1H), 7.89 – 7.81 (m, 1H), 7.72-7.65 (m, 1H), 7.60 – 7.52 (m, 1H), 7.49 – 7.40 (m, 1H), 7.05 (dd, *J* = 3.9, 0.9 Hz, 1H), 6.92 (dd, *J* = 3.8, 2.8 Hz, 1H), 4.15 (q, *J* = 7.1 Hz, 2H), 0.92 (t, *J* = 7.1 Hz, 3H).

^{13}C NMR (125MHz, $CDCl_3$) δ 167.0, 154.6, 152.6, 148.1, 139.3, 135.7, 131.7, 130.3, 129.9, 128.5, 128.2, 127.6, 126.9, 126.0, 125.5, 125.3, 114.5, 113.8, 108.8, 61.5, 13.8.

HRMS (ESI) m/z calcd for $C_{23}H_{17}N_3O_2$ $[M+H]^+$ 368.1394, found 368.1400.

4-(5-methoxyquinolin-2-yl)pyrrolo[1,2-a]quinoxaline(3ca)



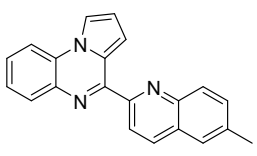
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 78% yield, 76.1 mg. m.p. 170-172 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.8 Hz, 1H), 8.59 (d, *J* = 8.8 Hz, 1H), 8.13 (d, *J* = 7.9 Hz, 1H), 8.07 (dd, *J* = 4.0, 1.2 Hz, 1H), 8.05 – 8.00 (m, 1H), 7.88 (dd, *J* = 16.1, 8.3 Hz, 2H), 7.67 (t, *J* = 8.1 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.47 (t, *J* = 7.5 Hz, 1H), 7.05 – 6.97 (m, 1H), 6.91 (d, *J* = 7.7 Hz, 1H), 4.03 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.3, 155.2, 151.0, 148.4, 135.6, 131.4, 130.4, 129.6, 128.2, 127.8, 125.2, 124.8, 122.2, 120.8, 119.8, 114.7, 114.5, 113.8, 111.5, 105.0, 55.8.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3O$ $[M+H]^+$ 326.1288, found 326.1294.

4-(6-methylquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3da)[S3]



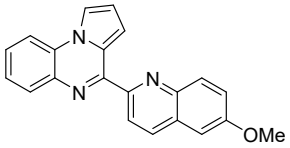
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 71% yield, 65.8 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.6 Hz, 1H), 8.24 (d, *J* = 8.6 Hz, 1H), 8.18 (d, *J* = 8.5 Hz, 1H), 8.14-8.07 (m, 2H), 8.04 (dd, *J* = 2.7, 1.3 Hz, 1H), 7.91 (dd, *J* = 8.2, 1.1

Hz, 1H), 7.65 (s, 1H), 7.61 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.58 – 7.52 (m, 1H), 7.48 (td, *J* = 7.7, 1.3 Hz, 1H), 7.01 (dd, *J* = 4.0, 2.7 Hz, 1H), 2.59 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.3, 151.1, 146.2, 137.4, 135.8, 135.6, 131.9, 130.4, 129.8, 128.4, 128.2, 127.8, 126.5, 125.2, 124.8, 120.7, 114.7, 114.4, 113.7, 111.4, 21.8.

4-(6-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ea)



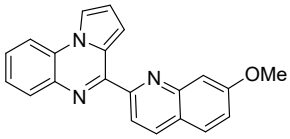
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 65% yield, 63.4 mg. m.p. 163-165 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.6 Hz, 1H), 8.22 – 8.15 (m, 2H), 8.12-8.08 (m, 2H), 8.04 – 7.98 (m, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.56 – 7.49 (m, 1H), 7.49 – 7.40 (m, 2H), 7.12 (d, *J* = 2.7 Hz, 1H), 7.00 (dd, *J* = 3.8, 2.8 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.5, 153.8, 151.0, 143.6, 135.7, 135.1, 131.6, 130.3, 129.5, 128.0, 127.7, 125.1, 124.7, 122.4, 121.0, 114.6, 114.3, 113.7, 111.4, 105.1, 55.6.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3O$ $[M+H]^+$ 326.1288, found 326.1295.

4-(7-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3fa)



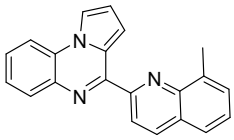
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 66% yield, 64.4 mg. m.p. 157-159 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.43 (d, *J* = 8.4 Hz, 1H), 8.23 (d, *J* = 8.4 Hz, 1H), 8.10 (dd, *J* = 8.0, 1.3 Hz, 1H), 8.01 (ddd, *J* = 5.3, 3.3, 1.2 Hz, 2H), 7.89 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.75 (d, J = 8.9 Hz, 1H), 7.58 (d, *J* = 2.4 Hz, 1H), 7.57 – 7.50 (m, 1H), 7.50 – 7.43 (m, 1H), 7.25 (dd, *J* = 5.3, 3.6 Hz, 1H), 7.00 (dd, *J* = 3.9, 2.7 Hz, 1H), 4.01 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 160.9, 156.3, 151.3, 149.3, 136.2, 135.7, 130.5, 128.6, 128.2, 127.7, 125.2, 124.8, 123.6, 120.6, 118.7, 114.6, 114.4, 113.7, 111.1, 107.9, 55.7.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3O$ $[M+H]^+$ 326.1288, found 326.1287.

4-(8-methylquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ga)



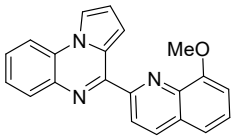
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 78% yield, 72.3 mg. m.p. 160-162 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.77 (d, *J* = 8.6 Hz, 1H), 8.31 – 8.28 (m, 2H), 8.13 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.05 (dd, *J* = 2.6, 1.3 Hz, 1H), 7.92 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.74 (d, *J* = 8.1 Hz, 1H), 7.64 (d, *J* = 6.9 Hz, 1H), 7.59 – 7.53 (m, 1H), 7.50-7.46 (m, 2H), 7.04 (dd, *J* = 3.9, 2.7 Hz, 1H), 3.01 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 154.80, 150.80, 146.79, 138.05, 136.58, 135.52, 130.41, 129.75, 128.39, 128.25, 127.79, 127.13, 125.65, 125.16, 124.68, 120.28, 114.68, 114.33, 113.70, 111.66, 18.84.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3$ $[M+H]^+$ 310.1339, found 310.1345.

4-(8-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ha)



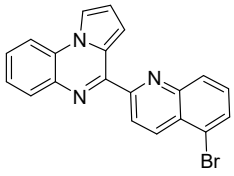
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 70% yield, 68.3 mg. m.p. 178-180 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 (d, *J* = 8.6 Hz, 1H), 8.37 (dd, *J* = 4.0, 1.2 Hz, 1H), 8.29 (d, *J* = 8.6 Hz, 1H), 8.12 (d, *J* = 7.9 Hz, 1H), 8.03 (dd, *J* = 2.6, 1.3 Hz, 1H), 7.90 (dd, *J* = 8.2, 0.9 Hz, 1H), 7.54-7.50 (m, 2H), 7.47-7.43 (m, 2H), 7.10 (d, J = 7.6 Hz, 1H), 7.04 (dd, *J* = 3.9, 2.7 Hz, 1H), 4.16 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 154.6, 150.8, 139.5, 136.3, 135.6, 130.4, 129.5, 128.2, 127.9, 127.7, 125.1, 124.9, 120.9, 119.3, 115.0, 114.3, 113.7, 111.9, 107.8, 56.2.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3O$ $[M+H]^+$ 326.1288, found 326.1294.

4-(5-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ia)



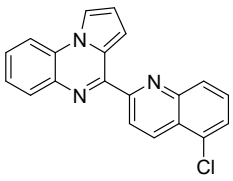
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 88% yield, 98.7 mg. m.p. 185-187 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.8 Hz, 1H), 8.65 (d, *J* = 8.9 Hz, 1H), 8.24 (d, *J* = 8.4 Hz, 1H), 8.13-8.08 (m, 2H), 8.03 (d, *J* = 1.2 Hz, 1H), 7.88 (dd, *J* = 15.1, 7.5 Hz, 2H), 7.66 – 7.58 (m, 1H), 7.58 – 7.52 (m, 1H), 7.52 – 7.43 (m, 1H), 7.01 (dd, *J* = 3.9, 2.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.6, 150.0, 148.3, 135.8, 135.4, 131.0, 130.5, 130.0, 129.8, 128.5, 127.7, 127.7, 125.3, 124.6, 121.9, 121.8, 114.8, 114.6, 113.7, 111.5.

HRMS (ESI) m/z calcd for $C_{20}H_{12}BrN_3$ $[M+H]^+$ 374.0287, found 374.0292.

4-(5-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ja)



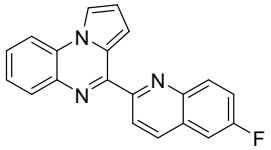
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 90% yield, 88.8 mg. m.p. 224-226 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.6 Hz, 1H), 8.23 (dd, *J* = 13.5, 8.8 Hz, 2H), 8.16 (d, *J* = 7.9 Hz, 1H), 8.11 (dd, *J* = 4.0, 1.1 Hz, 1H), 8.09 – 8.04 (m, 1H), 7.93 (d, *J* = 7.5 Hz, 1H), 7.88 (d, *J* = 2.2 Hz, 1H), 7.72 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.64 – 7.55 (m, 1H), 7.54 – 7.47 (m, 1H), 7.05-7.02 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.1, 150.3, 145.9, 135.5, 135.2, 133.2, 131.7, 130.6, 130.3, 128.9, 128.5, 127.7, 126.4, 125.3, 124.5, 121.6, 114.9, 114.8, 113.8, 111.7.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0801.

4-(6-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ka)[S5]



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 80% yield, 75.1 mg.

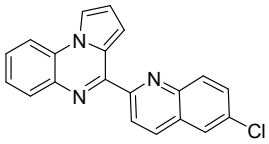
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.67 (d, *J* = 8.7 Hz, 1H), 8.32 – 8.21 (m, 2H), 8.13 – 8.06 (m, 2H), 8.06 – 8.00 (m, 1H), 7.91 (d, *J* = 8.2 Hz, 1H), 7.61 – 7.51 (m, 2H), 7.51 – 7.44 (m, 2H), 7.03-7.00 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 161.0 (d, *J* = 249.6 Hz), 155.5 (d, *J* = 2.1 Hz), 150.5, 144.6, 135.8 (d, *J* = 5.4 Hz), 135.5, 132.6 (d, *J* = 9.3 Hz), 130.4, 129.0 (d, *J* = 10.2 Hz), 128.4, 127.7, 125.3, 124.6, 121.4,

119.9 (d, *J* = 25.7 Hz), 114.7, 114.5, 113.8, 111.3, 110.8 (d, *J* = 21.8 Hz).

^{19}F NMR (470 MHz, $CDCl_3$) δ -112.00.

4-(6-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3la)



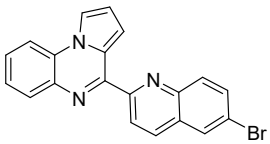
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 84% yield, 82.9 mg. m.p. 227-229 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.71 (d, *J* = 8.5 Hz, 1H), 8.23 (dd, *J* = 12.8, 9.0 Hz, 2H), 8.15 (d, *J* = 7.7 Hz, 1H), 8.11 (d, *J* = 3.0 Hz, 1H), 8.06 (s, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.88 (s, 1H), 7.71 (d, *J* = 8.6 Hz, 1H), 7.58 (t, *J* = 7.5 Hz, 1H), 7.50 (t, *J* = 7.5 Hz, 1H), 7.03 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 150.3, 145.9, 135.5, 135.2, 133.2, 131.7, 130.6, 130.3, 128.9, 128.5, 127.7, 126.4, 125.3, 124.5, 121.6, 114.9, 114.8, 113.8, 111.7.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0800.

4-(6-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ma)



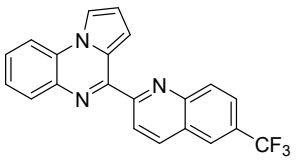
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 84% yield, 94.2 mg. m.p. 226-228 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.74 – 8.62 (m, 1H), 8.25 – 8.18 (m, 1H), 8.13 (d, *J* = 8.9 Hz, 2H), 8.10 (dd, *J* = 3.9, 1.2 Hz, 1H), 8.06 – 8.03 (m, 2H), 7.94 – 7.88 (m, 1H), 7.88 – 7.79 (m, 1H), 7.63 – 7.54 (m, 1H), 7.52 – 7.43 (m, 1H), 7.02 (dd, *J* = 3.9, 2.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 150.2, 146.1, 135.4, 135.3, 133.1, 131.7, 130.3, 129.7, 129.4, 128.5, 127.7, 125.3, 124.5, 121.6, 121.4, 114.9, 114.7, 113.8, 111.7.

HRMS (ESI) m/z calcd for $C_{20}H_{12}BrN_3$ $[M+H]^+$ 374.0287, found 374.0296.

4-(6-(trifluoromethyl)quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3na)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 95% yield, 103.5 mg. m.p. 165-167 ℃.

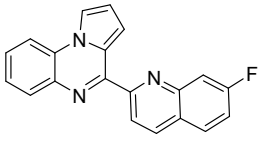
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.75 (d, *J* = 8.6 Hz, 1H), 8.35 (dd, *J* = 8.6, 3.9 Hz, 2H), 8.16 (s, 1H), 8.11 (dd, *J* = 4.0, 1.1 Hz, 1H), 8.08 (dd, *J* = 8.0, 1.1 Hz, 1H), 8.04 – 7.99 (m, 1H), 7.92 (dd, *J* = 8.8, 1.8 Hz, 1H), 7.88 (d, *J* = 8.2 Hz, 1H), 7.59 – 7.52 (m, 1H), 7.50 – 7.44 (m, 1H), 7.01 (dd, *J* = 3.9, 2.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 158.1, 149.9, 148.5, 137.0, 135.4, 131.2, 130.5, 128.9 (q, *J* = 32.7 Hz), 128.6, 127.8, 127.2, 125.6 (q, *J* = 4.4 Hz), 125.3, 125.2 (q, *J* = 2.9 Hz), 124.5, 124.0 (q, *J* = 272.4 Hz), 121.8, 114.8, 114.5, 113.7, 111.4.

^{19}F NMR (470 MHz, $CDCl_3$) δ -62.11.

HRMS (ESI) m/z calcd for $C_{21}H_{12}F_3N_3$ $[M+H]^+$ 364.1056, found 364.1065.

4-(7-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3oa)[S3]



The title compound was prepared according to the general working

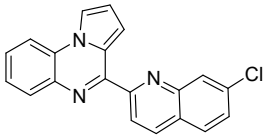
procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 83% yield, 77.9 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.58 (d, *J* = 8.6 Hz, 1H), 8.25 (d, *J* = 8.6 Hz, 1H), 8.10 – 8.04 (m, 2H), 8.02 – 7.96 (m, 1H), 7.92 – 7.81 (m, 3H), 7.56 – 7.49 (m, 1H), 7.49 – 7.41 (m, 1H), 7.36 (td, *J* = 8.6, 2.5 Hz, 1H), 6.99 (dd, *J* = 3.9, 2.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 163.2 (d, *J* = 249.9 Hz), 157.1, 150.4, 148.4 (d, *J* = 12.6 Hz), 136.2, 135.6, 130.5, 129.5 (d, *J* = 9.7 Hz), 128.4, 127.8, 125.3, 125.1, 124.6, 120.0 (d, *J* = 2.5 Hz), 117.7 (d, *J* = 25.6 Hz), 114.6, 114.4, 113.7, 113.6 (d, *J* = 20.1 Hz), 111.3.

^{19}F NMR (470 MHz, $CDCl_3$) δ -109.66.

4-(7-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3pa)



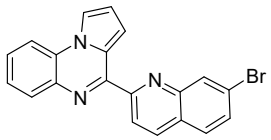
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 90% yield, 88.8 mg. m.p. 215-217 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.68 (d, *J* = 8.6 Hz, 1H), 8.34-8.27 (m, 2H), 8.15 (d, *J* = 7.9 Hz, 1H), 8.13 – 8.08 (m, 1H), 8.06 (d, *J* = 1.2 Hz, 1H), 7.93 (d, *J* = 8.1 Hz, 1H), 7.83 (d, *J* = 8.7 Hz, 1H), 7.63 – 7.54 (m, 2H), 7.50 (t, *J* = 7.2 Hz, 1H), 7.03 (dd, *J* = 3.7, 2.9 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.8, 149.2, 146.9, 135.2, 134.4, 134.2, 129.3, 128.0, 127.8, 127.5, 127.3, 126.7, 125.7, 124.3, 123.5, 119.9, 113.8, 113.7, 112.8, 110.7.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0802.

4-(7-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3qa)



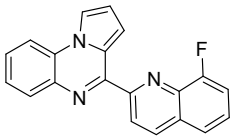
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 83% yield, 92.8 mg. m.p. 198-200 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.72 (d, *J* = 8.6 Hz, 1H), 8.48 (d, *J* = 1.9 Hz, 1H), 8.31 (d, *J* = 8.5 Hz, 1H), 8.17 (d, *J* = 7.9 Hz, 1H), 8.13 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.07 (dd, *J* = 2.7, 1.3 Hz, 1H), 7.93 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.77 (d, *J* = 8.6 Hz, 1H), 7.70 (dd, *J* = 8.6, 1.9 Hz, 1H), 7.62 – 7.55 (m, 1H), 7.53 – 7.47 (m, 1H), 7.04 (dd, *J* = 4.0, 2.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.8, 150.0, 148.2, 136.3, 134.2, 132.4, 130.9, 130.3, 128.9, 128.6, 127.7, 127.0, 125.4, 124.5, 123.7, 121.2, 115.0, 114.9, 113.8, 112.0.

HRMS (ESI) m/z calcd for $C_{20}H_{12}BrN_3$ $[M+H]^+$ 374.0287, found 374.0290.

4-(8-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ra)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 84% yield, 78.9 mg. m.p. 220-222 ℃.

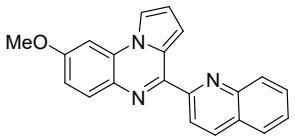
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.7 Hz, 1H), 8.43 – 8.32 (m, 2H), 8.19 (d, *J* = 7.8 Hz, 1H), 8.08 (dd, *J* = 2.6, 1.2 Hz, 1H), 7.94 (dd, *J* = 8.2, 1.0 Hz, 1H), 7.69 (d, *J* = 8.1 Hz, 1H), 7.52 (m, 4H), 7.60-7.44 (dd, *J* = 4.0, 2.7 Hz, 1H).

^{13}C NMR (125 MHz, THF) δ 158.7 (d, *J* = 257.4 Hz), 156.1, 149.2, 137.6 (d, *J* = 12.0 Hz), 135.6 (d, *J* = 3.1 Hz), 135.5, 130.3, 130.0 (d, *J* = 1.4 Hz), 128.4, 128.1, 127.1 (d, *J* = 8.1 Hz), 124.8, 124.2, 123.3, 123.2, 120.8, 114.5 (d, *J* = 39.7 Hz), 114.0, 113.4 (d, *J* = 18.5 Hz), 112.2.

^{19}F NMR (470 MHz, $CDCl_3$) δ -124.26.

HRMS (ESI) m/z calcd for $C_{20}H_{12}FN_3$ $[M+H]^+$ 314.1088, found 314.1091.

8-methoxy-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ab)[S4]

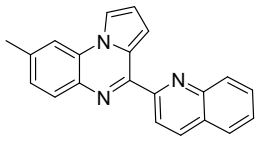


The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 79% yield, 77.7 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.5 Hz, 1H), 8.29 (t, *J* = 9.1 Hz, 2H), 8.11 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.04 (d, *J* = 8.9 Hz, 1H), 7.92 (dd, *J* = 2.7, 1.3 Hz, 1H), 7.90 – 7.84 (m, 1H), 7.79-7.75 (m, 1H), 7.63 – 7.54 (m, 1H), 7.29 (d, *J* = 2.6 Hz, 1H), 7.07 (dd, *J* = 8.9, 2.6 Hz, 1H), 7.01 (dd, *J* = 3.9, 2.8 Hz, 1H), 3.97 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 159.85 (s), 156.26 (s), 148.35 (s), 147.61 (s), 136.29 (s), 131.74 (s), 130.06 (s), 130.01 (s), 129.53 (s), 128.61 (s), 128.21 (s), 127.62 (s), 127.15 (s), 124.66 (s), 120.55 (s), 114.77 (s), 113.89 (s), 113.05 (s), 110.89 (s), 97.40 (s), 55.83.

8-methyl-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ac)



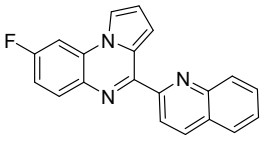
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 81% yield, 75.8 mg. m.p. 153-155 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.66 (d, *J* = 8.6 Hz, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 8.28 (d, *J* = 8.4 Hz, 1H), 8.13 – 8.06 (m, 2H), 8.01 (d, *J* = 1.2 Hz, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.81 – 7.73 (m, 1H), 7.69 (s, 1H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.29 (d, *J* = 8.2 Hz, 1H), 7.01 (dd, *J* = 3.8, 2.8 Hz, 1H), 2.56 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.4, 149.6, 147.6, 139.2, 136.5, 132.7, 130.1, 129.7, 129.6, 128.4, 127.7, 127.4, 127.4, 126.8, 124.6, 120.9, 115.0, 114.8, 113.8, 112.1, 22.0.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3$ $[M+H]^+$ 310.1339, found 310.1346.

8-fluoro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ad)[S4]



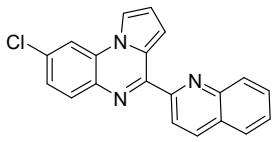
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 90% yield, 85.3 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.6 Hz, 1H), 8.29 (dd, *J* = 13.7, 8.5 Hz, 2H), 8.12 (dd, *J* = 4.0, 1.3 Hz, 1H), 8.09 (dd, *J* = 8.9, 5.9 Hz, 1H), 7.91 – 7.84 (m, 2H), 7.79-7.76 (m, 1H), 7.63-7.58 (m, 1H), 7.54 (dd, *J* = 9.2, 2.6 Hz, 1H), 7.19 (td, *J* = 8.6, 2.6 Hz, 1H), 7.01 (dd, *J* = 3.9, 2.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 162.0 (d, *J* = 249.4 Hz), 155.7, 150.0 (d, *J* = 2.7 Hz), 147.5, 136.4, 132.2 (d, *J* = 9.9 Hz), 132.1, 130.1, 129.7, 128.5 (d, *J* = 11.4 Hz), 128.3, 127.6, 127.4, 124.3, 120.5, 115.2, 114.7, 113.2 (d, *J* = 23.2 Hz), 111.9, 100.6 (d, *J* = 26.8 Hz).

^{19}F NMR (470 MHz, $CDCl_3$) δ -109.53.

8-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ae)



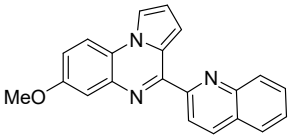
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 92% yield, 91.6 mg. m.p. 212-214 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 8.6 Hz, 1H), 8.30 (dd, *J* = 19.9, 8.5 Hz, 2H), 8.14 (d, *J* = 2.9 Hz, 1H), 8.03 (d, *J* = 8.5 Hz, 1H), 7.95 (s, 1H), 7.89 (d, *J* = 8.2 Hz, 2H), 7.79 (t, *J* = 7.5 Hz, 1H), 7.62 (t, *J* = 7.4 Hz, 1H), 7.42 (d, *J* = 8.6 Hz, 1H), 7.03 (s, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.7, 150.9, 147.6, 136.4, 134.1, 133.7, 131.5, 130.1, 129.7, 128.4, 128.3, 127.6, 127.5, 125.6, 124.6, 120.5, 115.3, 114.7, 113.9, 112.1.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0796.

7-methoxy-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3af)



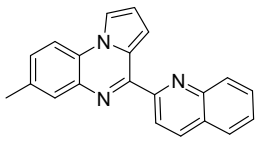
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 72% yield, 70.8 mg. m.p. 201-203 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 8.6 Hz, 1H), 8.33 (d, *J* = 8.6 Hz, 1H), 8.29 (d, *J* = 8.4 Hz, 1H), 8.05 (dd, *J* = 4.1, 1.3 Hz, 1H), 7.97 (dd, *J* = 2.6, 1.3 Hz, 1H), 7.90 (d, *J* = 7.3 Hz, 1H), 7.82 (d, *J* = 9.0 Hz, 1H), 7.81-7.76 (m, 1H), 7.64 – 7.55 (m, 2H), 7.18 (dd, *J* = 9.0, 2.8 Hz, 1H), 6.98 (dd, *J* = 4.0, 2.6 Hz, 1H), 3.95 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 157.2, 156.0, 151.2, 147.6, 136.6, 136.5, 130.2, 129.7, 128.3, 127.6, 127.4, 124.5, 122.1, 120.7, 117.7, 114.7, 114.5, 114.2, 111.4, 111.1, 55.8.

HRMS (ESI) m/z calcd for $C_{21}H_{15}N_3O$ $[M+H]^+$ 326.1288, found 326.1297.

7-methyl-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ag)[S4]

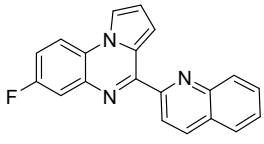


The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 93% yield, 87.1 mg.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.63 (d, *J* = 8.6 Hz, 1H), 8.31 (dd, *J* = 11.5, 8.6 Hz, 2H), 8.09 (dd, *J* = 3.9, 0.9 Hz, 1H), 7.99 (d, *J* = 1.2 Hz, 1H), 7.92 (s, 1H), 7.89 (d, *J* = 8.1 Hz, 1H), 7.81 – 7.74 (m, 2H), 7.60 (t, *J* = 7.4 Hz, 1H), 7.35 (dd, *J* = 8.3, 1.4 Hz, 1H), 6.99 (dd, *J* = 3.7, 2.8 Hz, 1H), 2.52 (s, 3H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.2, 150.8, 147.6, 136.4, 135.5, 135.0, 130.2, 130.1, 129.6, 129.5, 128.3, 127.6, 127.3, 125.6, 124.7, 120.7, 114.4, 114.2, 113.5, 111.2, 21.1.

7-fluoro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ah)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 85% yield, 80.6 mg. m.p. 170-172 ℃.

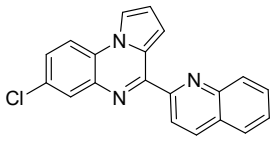
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.60 (d, *J* = 8.6 Hz, 1H), 8.30 (dd, *J* = 14.0, 8.6 Hz, 2H), 8.13 (dd, *J* = 4.0, 1.1 Hz, 1H), 7.99 – 7.93 (m, 1H), 7.88 (d, *J* = 8.1 Hz, 1H), 7.83 (dd, *J* = 9.0, 5.0 Hz, 1H), 7.80 – 7.74 (m, 2H), 7.64 – 7.57 (m, 1H), 7.29-7.23 (m, 1H), 7.01-6.97 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 159.8 (d, *J* = 243.7 Hz), 155.7, 151.8, 147.6, 136.7 (d, *J* = 11.4 Hz), 136.5, 130.1, 129.7, 128.4, 127.6, 127.5, 124.5, 124.4 (d, *J* = 1.9 Hz), 120.6, 115.9 (d, *J* = 24.6 Hz), 115.5 (d, *J* = 22.2 Hz), 114.9, 114.8, 114.7 (d, *J* = 17.0 Hz), 111.9.

^{19}F NMR (470 MHz, $CDCl_3$) δ -116.83.

HRMS (ESI) m/z calcd for $C_{20}H_{12}FN_3$ $[M+H]^+$ 314.1088, found 314.1097.

7-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ai)



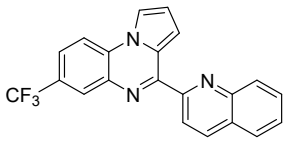
The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 87% yield, 86.7 mg. m.p. 202-204 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.61 (d, *J* = 8.6 Hz, 1H), 8.32 (d, *J* = 8.6 Hz, 1H), 8.28 (d, *J* = 8.4 Hz, 1H), 8.14 (dd, *J* = 4.0, 1.2 Hz, 1H), 8.10 (d, *J* = 2.2 Hz, 1H), 7.99 (dd, *J* = 2.6, 1.2 Hz, 1H), 7.89 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.75 (m, 2H), 7.66 – 7.58 (m, 1H), 7.49 (dd, *J* = 8.7, 2.3 Hz, 1H), 7.01 (dd, *J* = 4.0, 2.7 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.8, 151.8, 147.5, 136.6, 136.5, 130.2, 130.1, 129.8, 129.7, 128.4, 128.2, 127.7, 127.5, 126.4, 124.6, 120.6, 115.0, 114.9, 114.6, 112.0.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0802.

4-(quinolin-2-yl)-7-(trifluoromethyl)pyrrolo[1,2-*a*]quinoxaline(3aj)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 92% yield, 101.1 mg. m.p. 172-174 ℃.

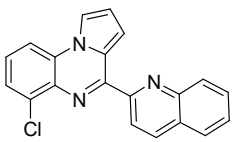
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.56 (d, *J* = 8.6 Hz, 1H), 8.30 (s, 1H), 8.24 (d, *J* = 8.4 Hz, 2H), 8.19 (dd, *J* = 3.9, 1.0 Hz, 1H), 7.94 (m, 1H), 7.84 (d, *J* = 8.3 Hz, 2H), 7.77 (m, 1H), 7.71 – 7.65 (m, 1H), 7.59 (t, *J* = 7.5 Hz, 1H), 6.99 (m, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 155.6, 151.8, 147.5, 136.3, 135.2, 130.1, 129.7, 129.6, 128.4, 127.9 (q, *J* = 3.4 Hz), 127.6, 127.5, 127.1 (q, *J* = 33.2 Hz), 124.7, 124.3 (q, *J* = 3.4 Hz), 124.0 (q, *J* = 271.8 Hz), 120.4, 115.5, 114.9, 114.3, 112.6.

^{19}F NMR (470 MHz, $CDCl_3$) δ -61.84.

HRMS (ESI) m/z calcd for $C_{21}H_{12}F_3N_3$ $[M+H]^+$ 364.1056, found 364.1064.

6-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ak)



The title compound was prepared according to the general working procedure and purified by column chromatography (petroleum ether/ethyl acetate = 10:1) to give the product as a yellow solid. 81% yield, 80.7 mg. m.p. 199-201 ℃.

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.83 (d, *J* = 8.6 Hz, 1H), 8.42 – 8.25 (m, 3H), 8.02 (dd, *J* = 2.5, 1.1 Hz, 1H), 7.90 (d, *J* = 8.1 Hz, 1H), 7.84 – 7.74 (m, 2H), 7.67 – 7.59 (m, 1H), 7.57 (dd, *J* = 7.8, 1.0 Hz, 1H), 7.44 (t, *J* = 8.1 Hz, 1H), 7.05 (dd, *J* = 3.9, 2.8 Hz, 1H).

^{13}C NMR (125 MHz, $CDCl_3$) δ 156.0, 150.5, 147.4, 136.5, 135.0, 132.7, 130.1, 129.6, 129.0, 128.5, 127.9, 127.7, 127.5, 125.8, 124.7, 120.9, 115.4, 115.0, 112.5, 112.2.

HRMS (ESI) m/z calcd for $C_{20}H_{12}ClN_3$ $[M+H]^+$ 330.0793, found 330.0802.

References

[S1] W. Bi, C. Qu, X. Chen, S. Wei, L. Qu, S. Liu, K. Sun, Y. Zhao, *Tetrahedron*, 2018, **74**, 1908-1917.

[S2] X. Zhang, X. Miao, Y. Zhou, Y. Wang, Y. Song, H. Liu, Y. Xiong, L. Li, A. Wu, Y. Zhu, *Org. Biomol. Chem.*, 2022, **20**, 1236-1242

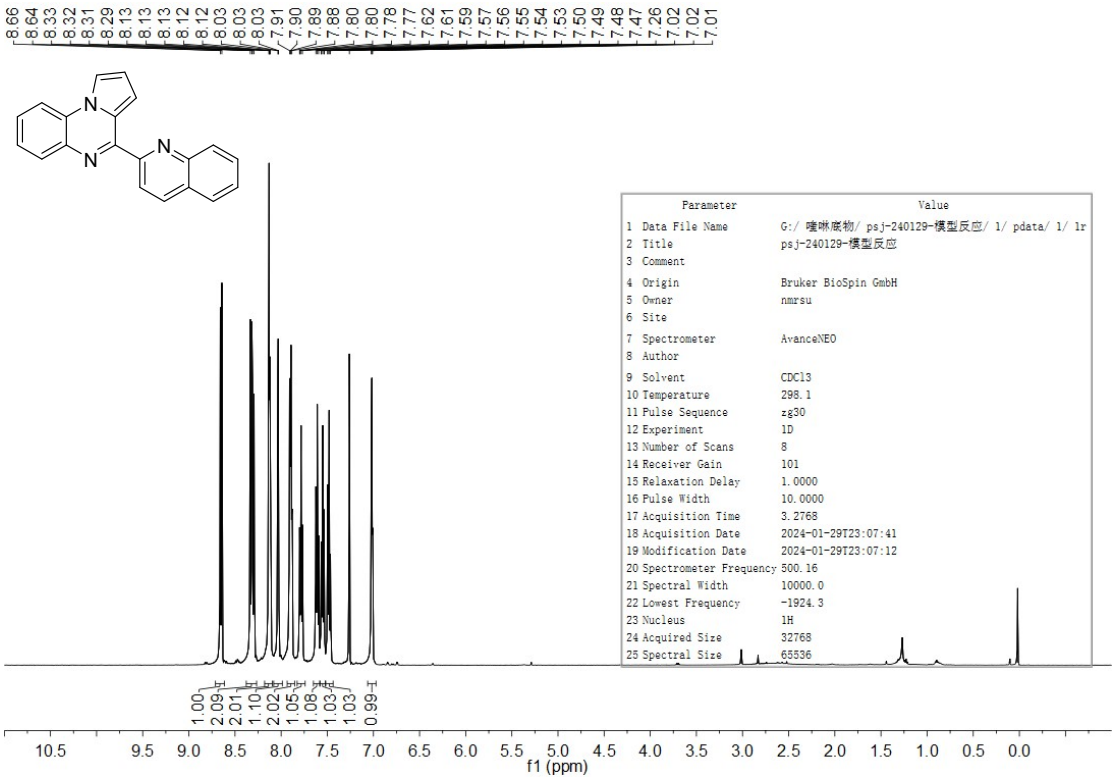
[S3] C. Dai, S. Deng, Q. Zhu and X. Tang, *RSC Adv.*, 2017, **7**, 44132-44135.

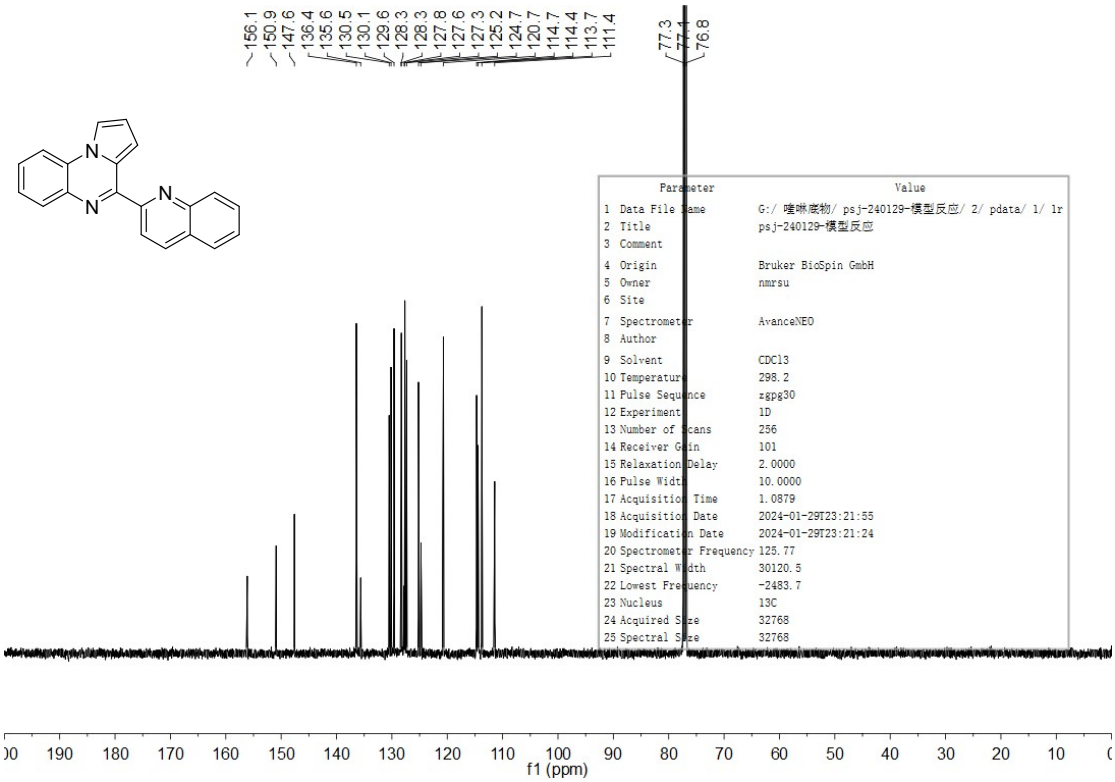
[S4] X. Pang, M. Wu, J. Ni, F. Zhang, J. Lan, B. Chen, and R. Yan, *J. Org. Chem.* 2017, **82,** 10110-10120.

[S5] B. Sridevi, S. Reddy Kandimalla and B. Subba Reddy, *Eur. J. Org. Chem.*, 2019, **40**, 6800-6806.

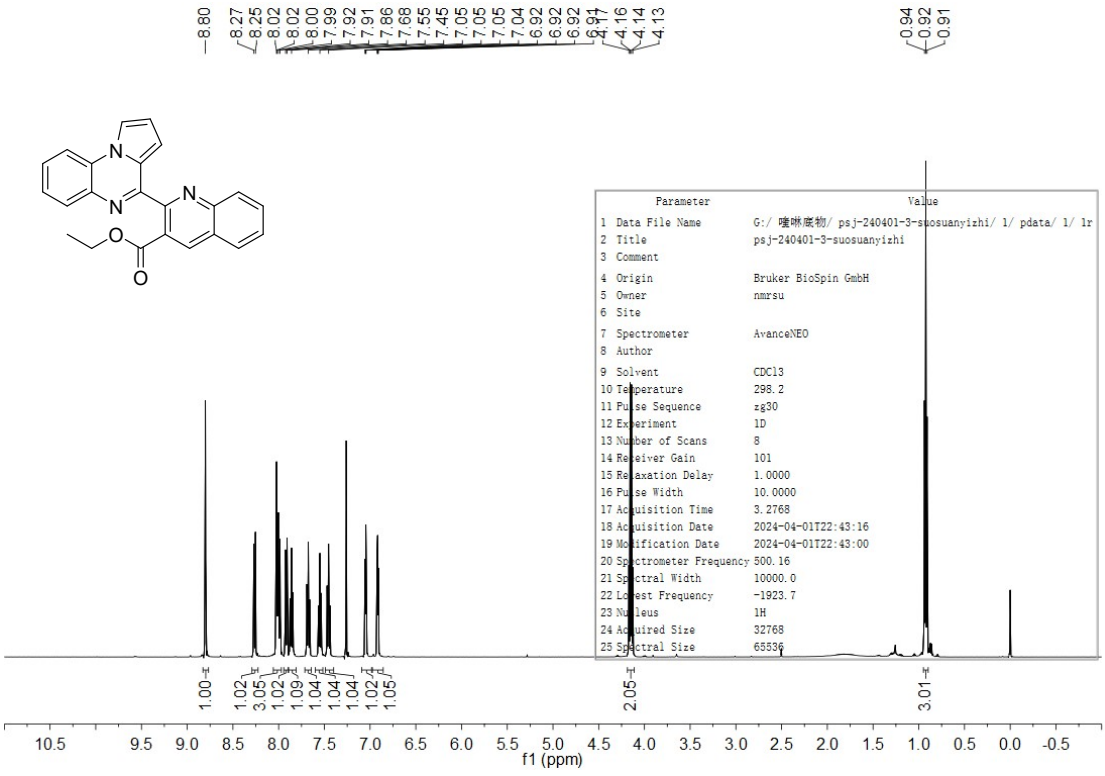
Copies of Product NMR Spectra

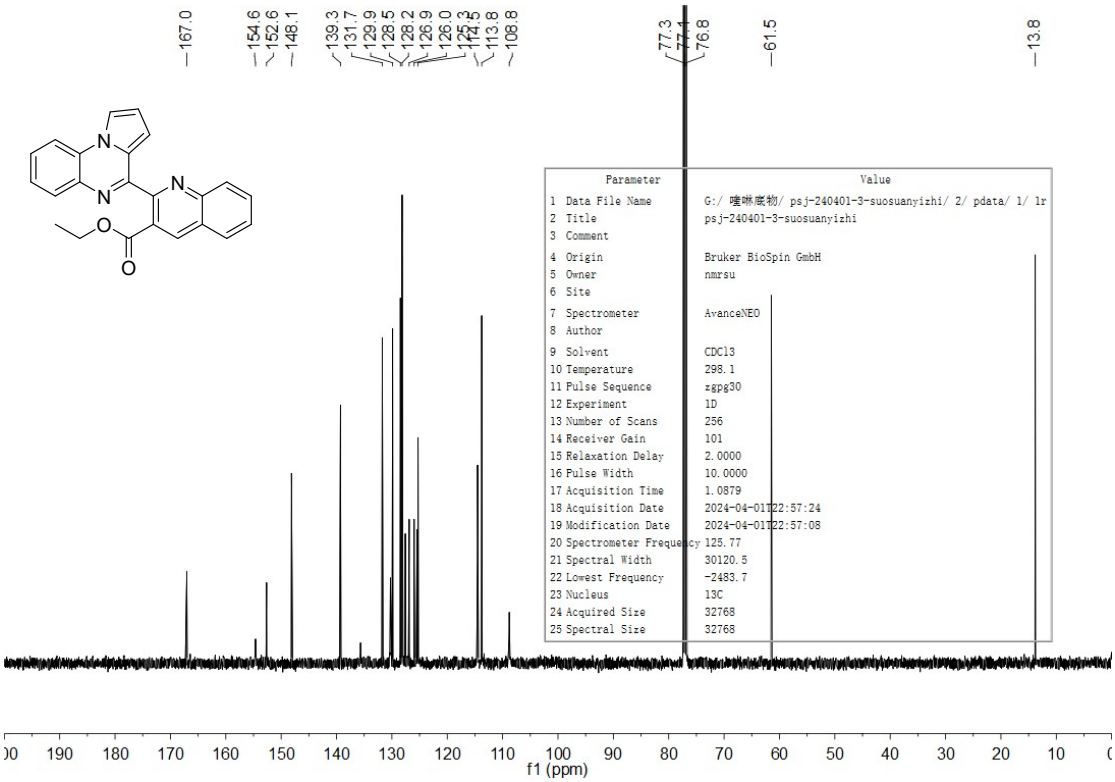
4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3aa)[S3]



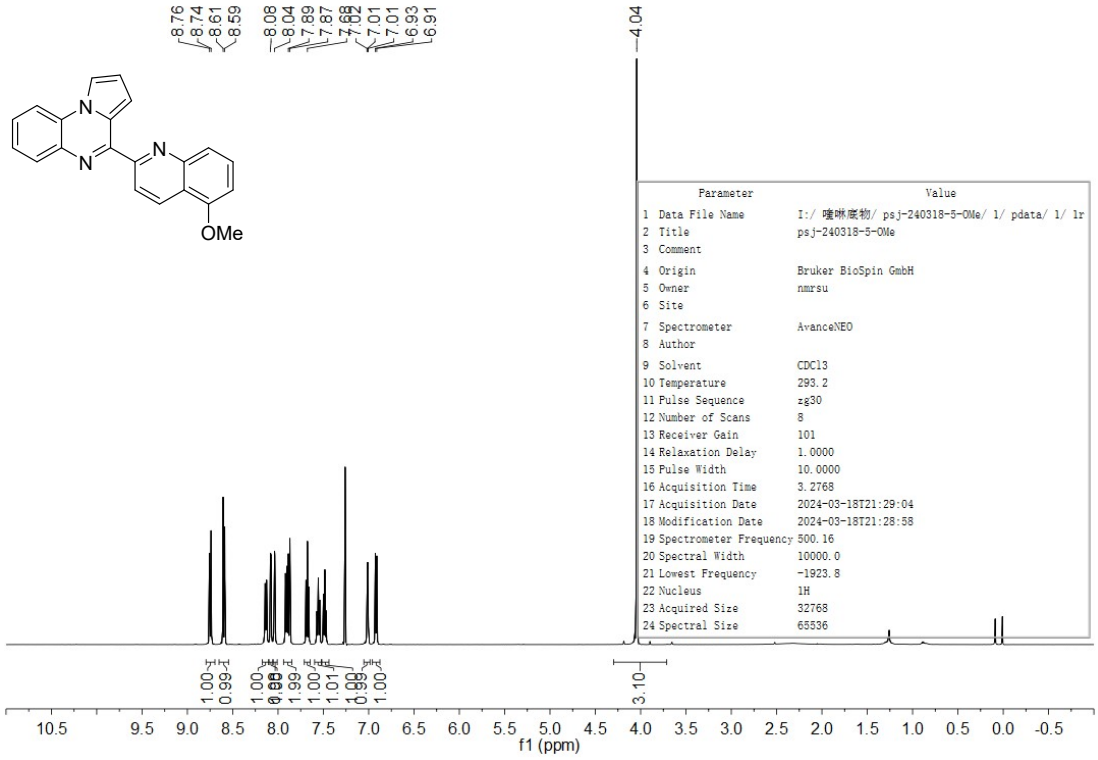


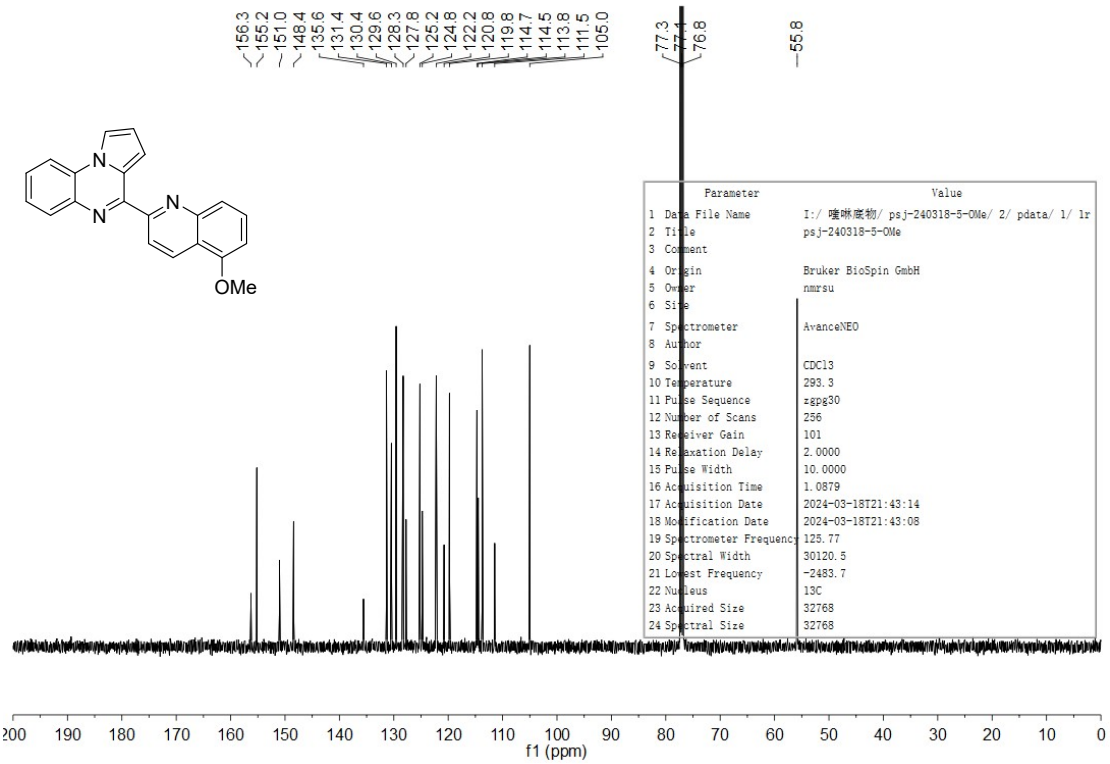
ethyl 2-(pyrrolo[1,2-*a*]quinoxalin-4-yl)quinoline-3-carboxylate(3ba)



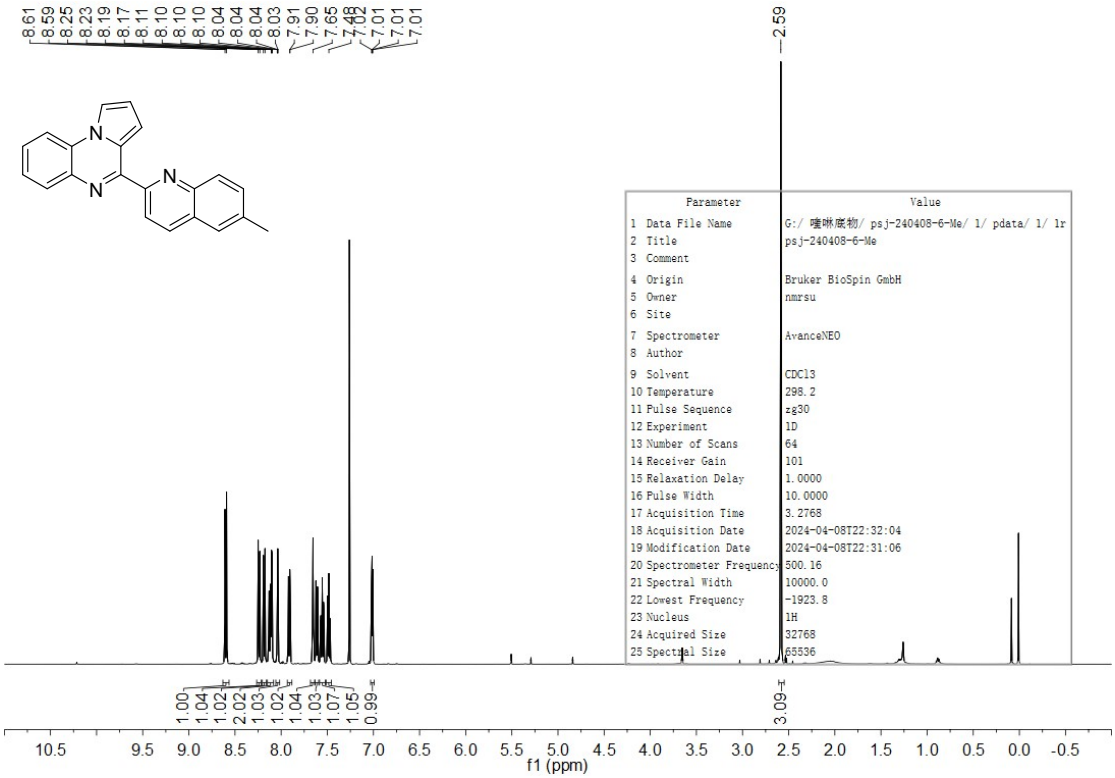


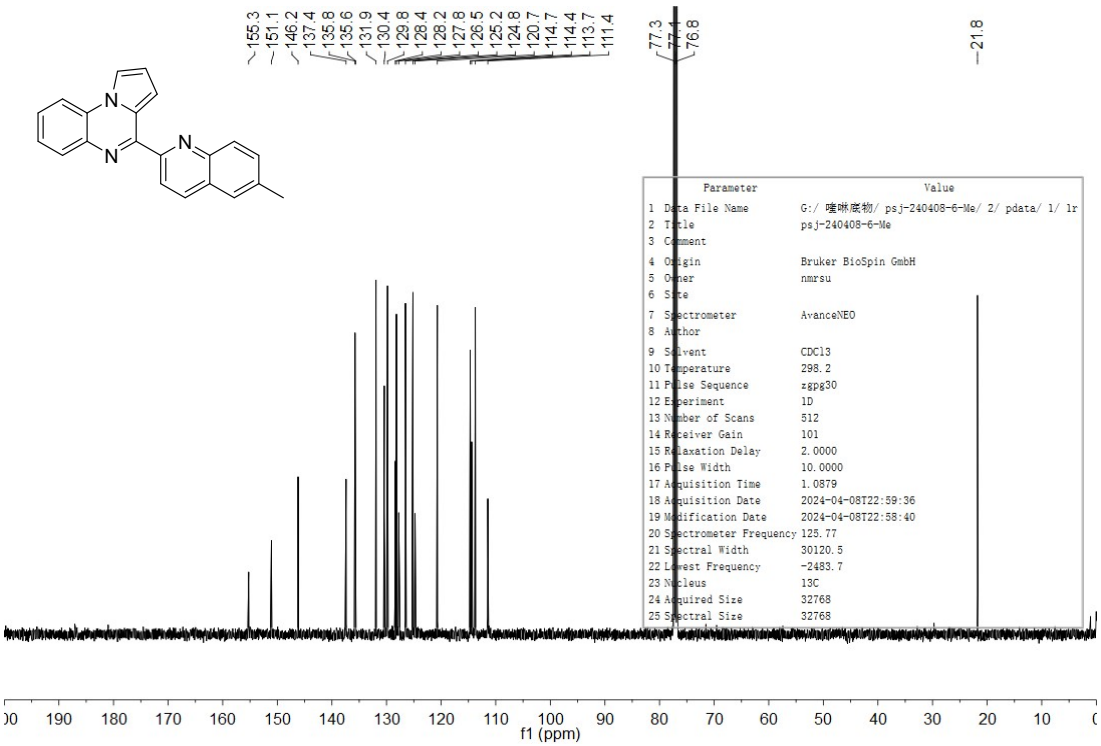
4-(5-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ca)



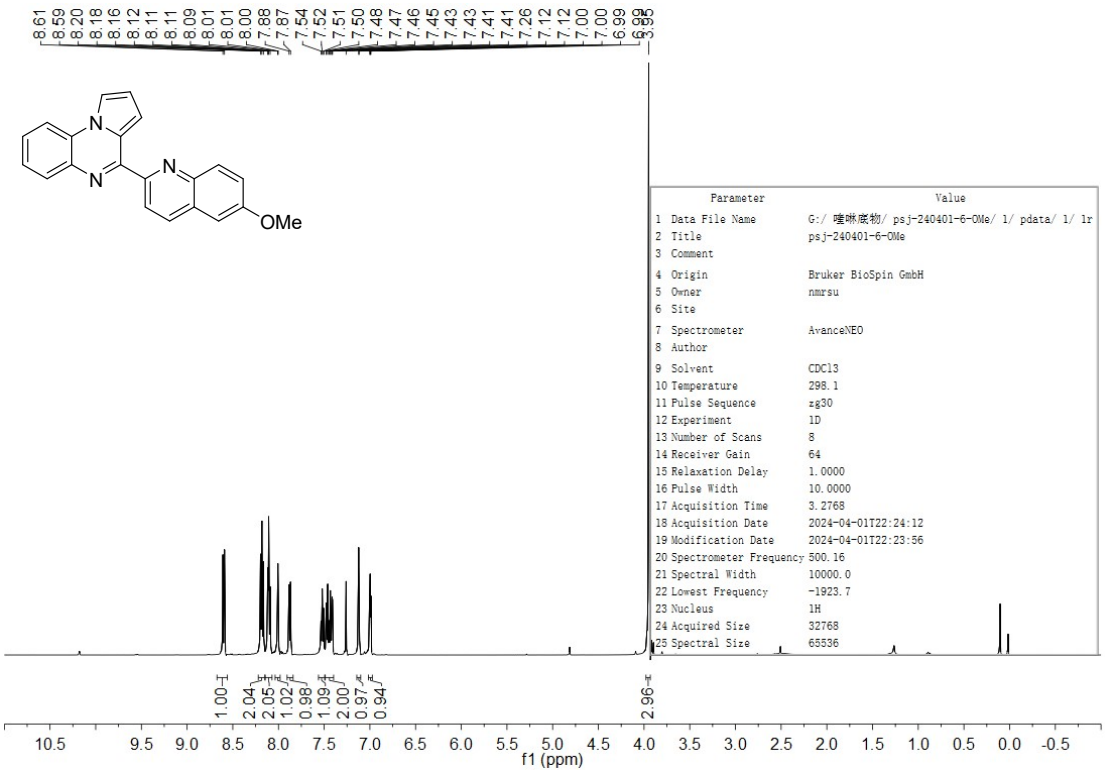


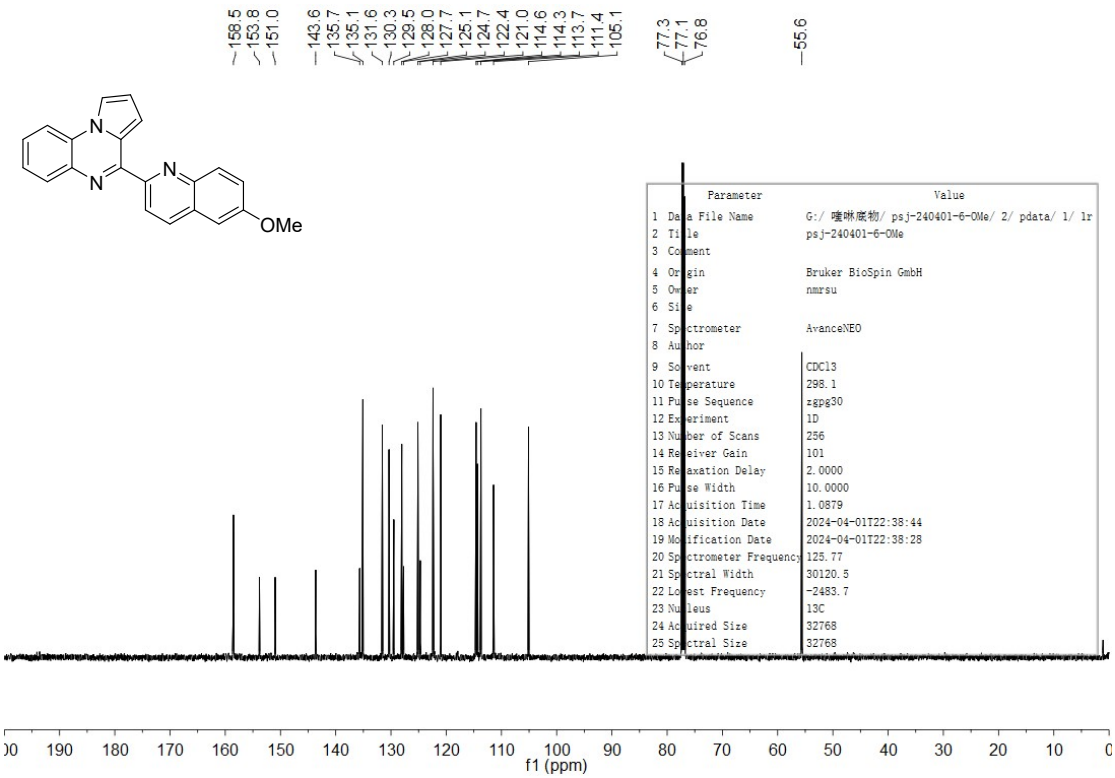
4-(6-methylquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3da)[S3]



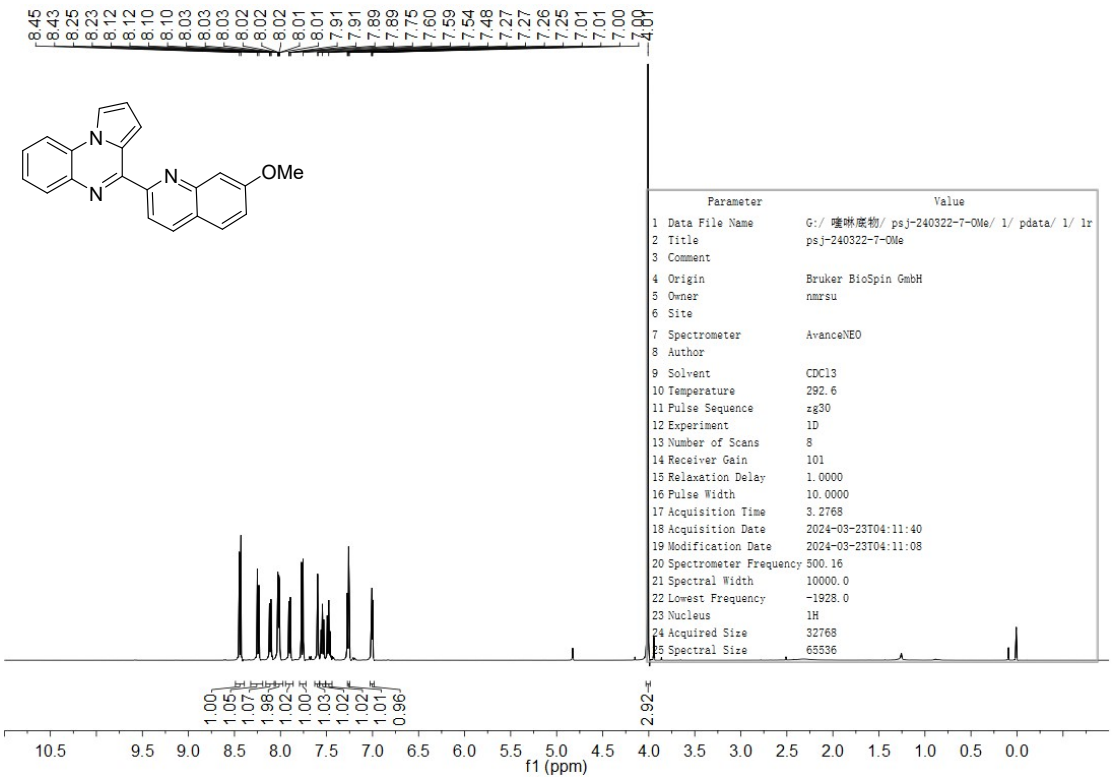


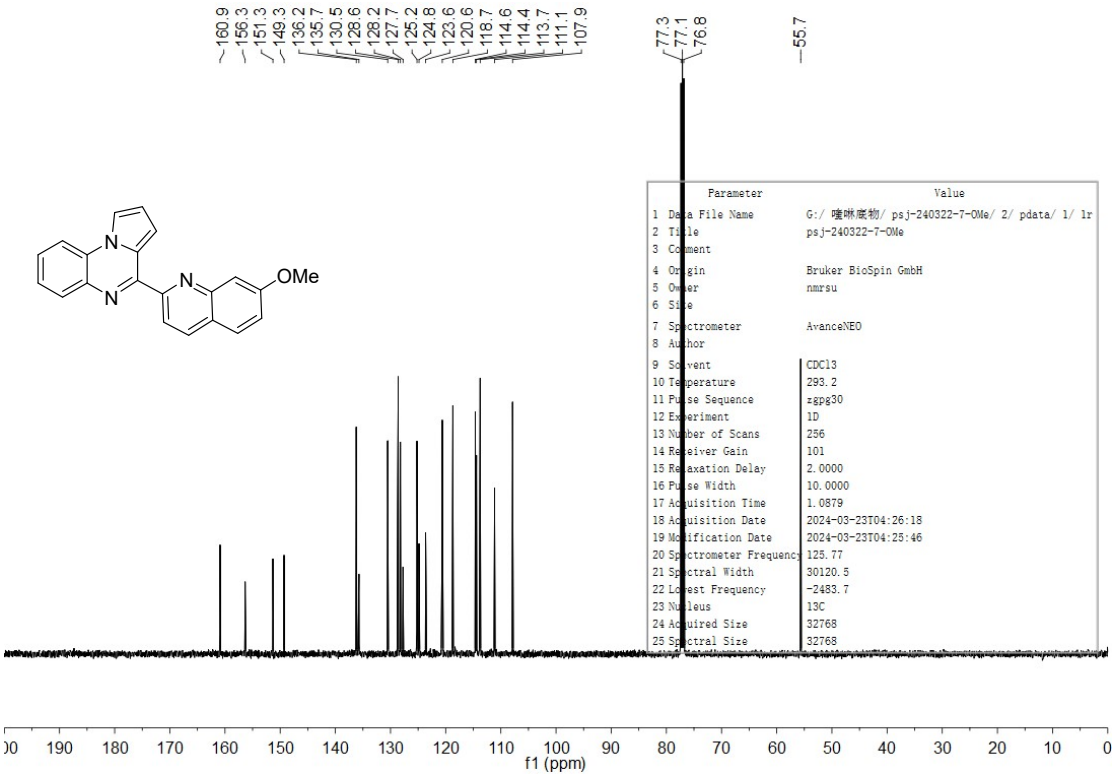
4-(6-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ea)





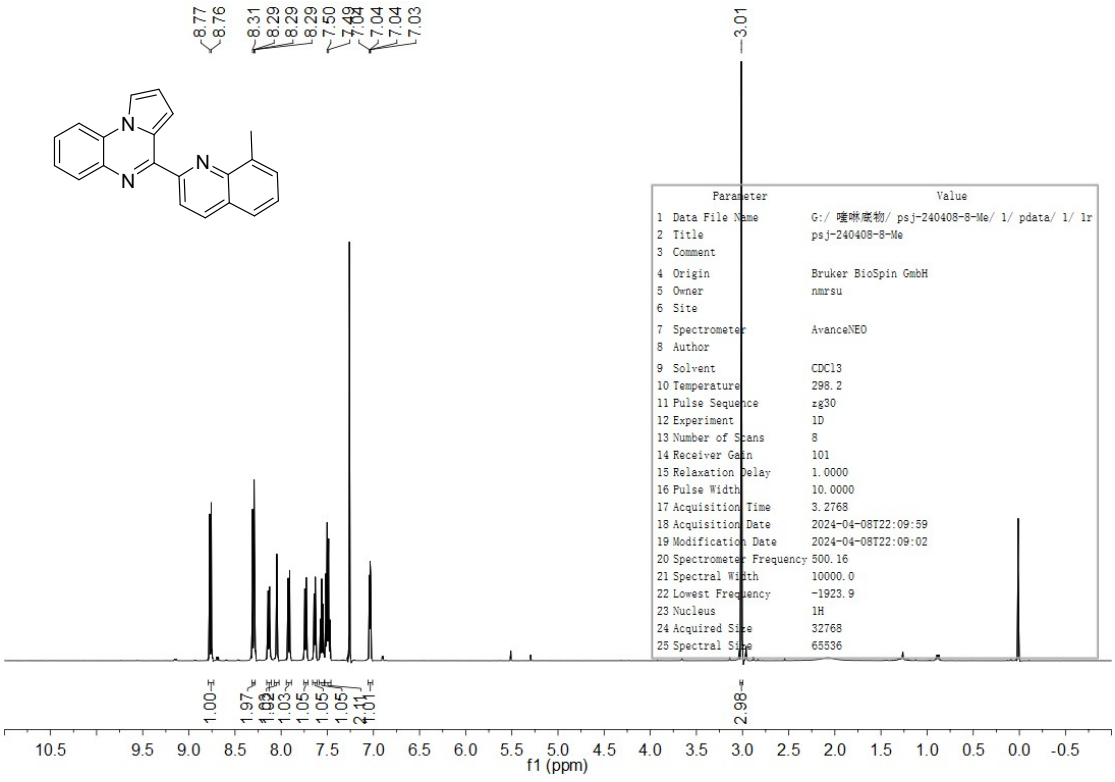
4-(7-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3fa)



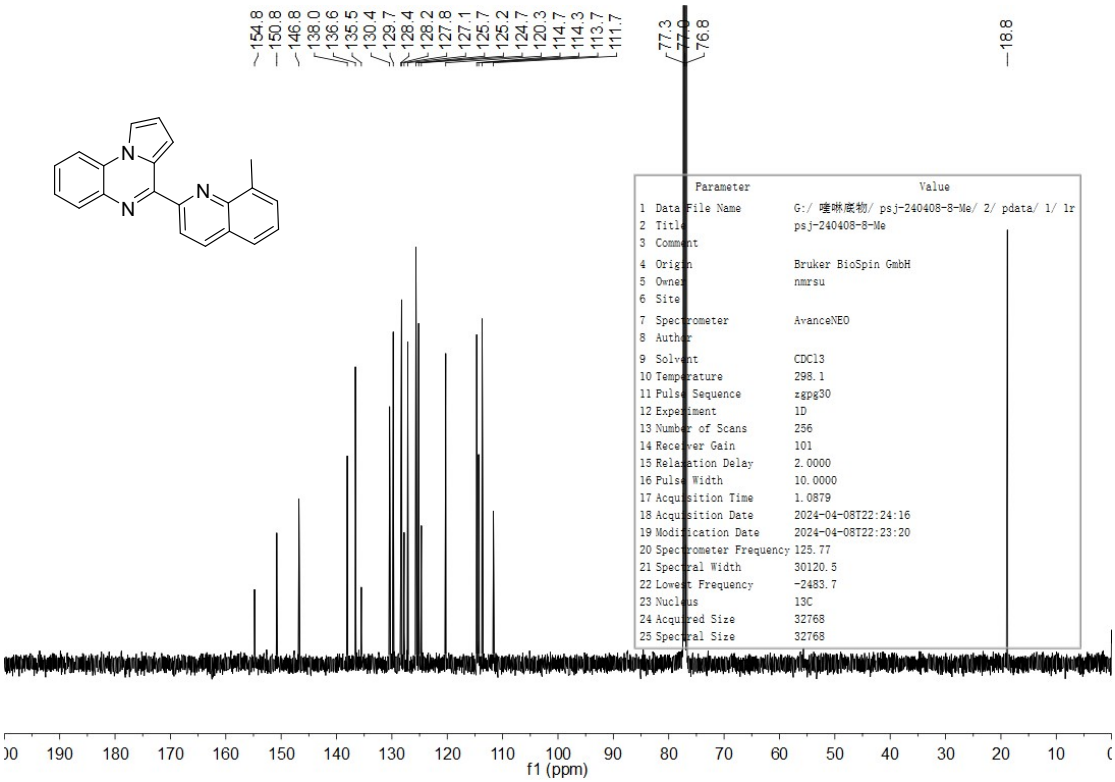


Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240322-7-OMe/ 2/ pdata/ 1/ 1r
2 Title	psj-240322-7-OMe
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.2
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-03-23T04:26:18
19 Modification Date	2024-03-23T04:25:46
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2483.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

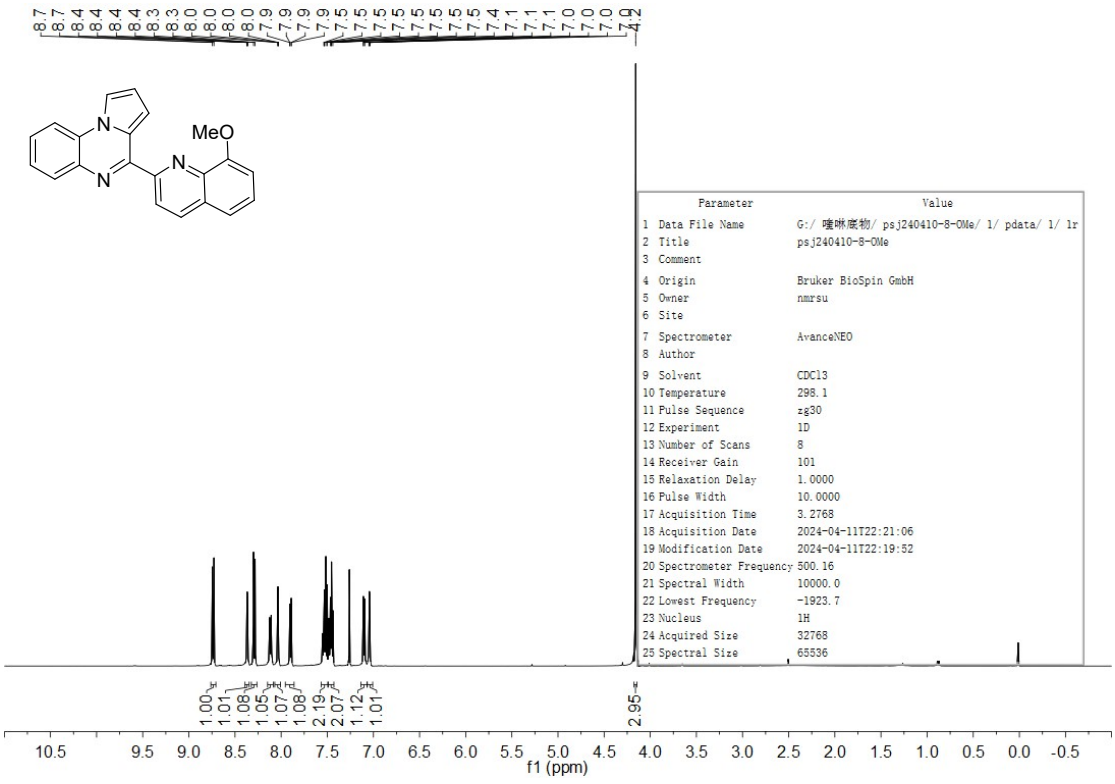
4-(8-methylquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ga)

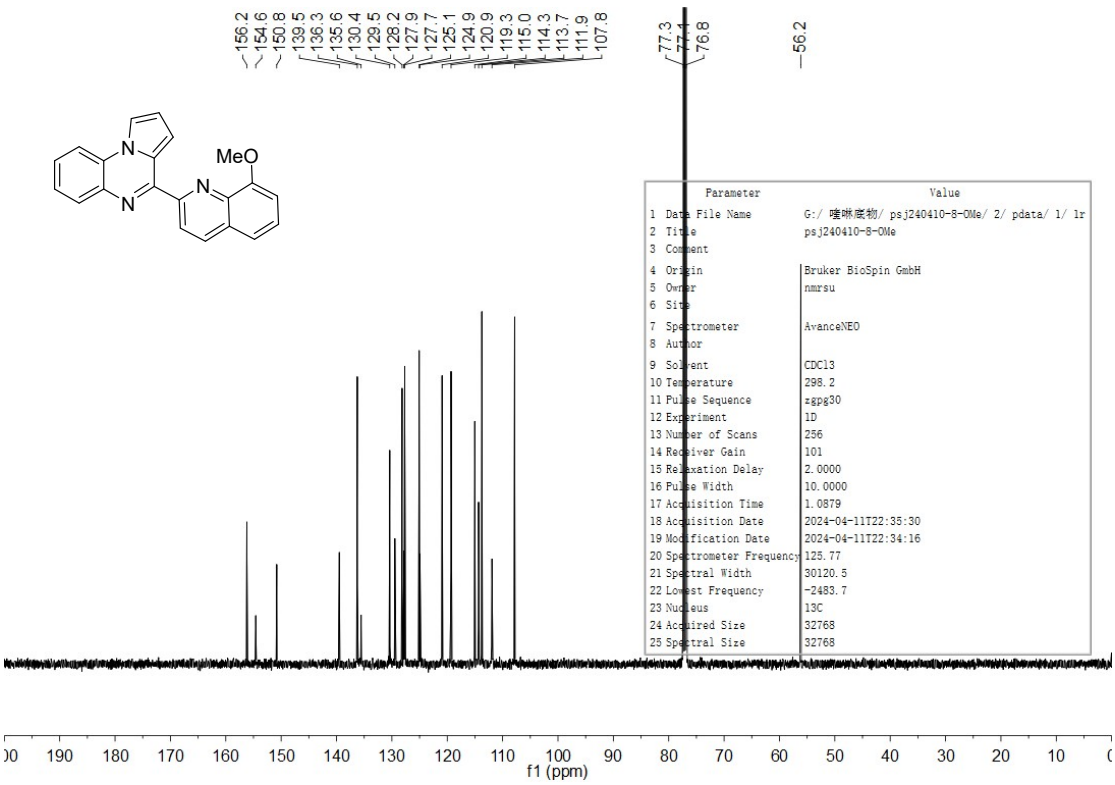


Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240408-8-Me/ 1/ pdata/ 1/ 1r
2 Title	psj-240408-8-Me
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-04-08T22:09:59
19 Modification Date	2024-04-08T22:09:02
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1923.9
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

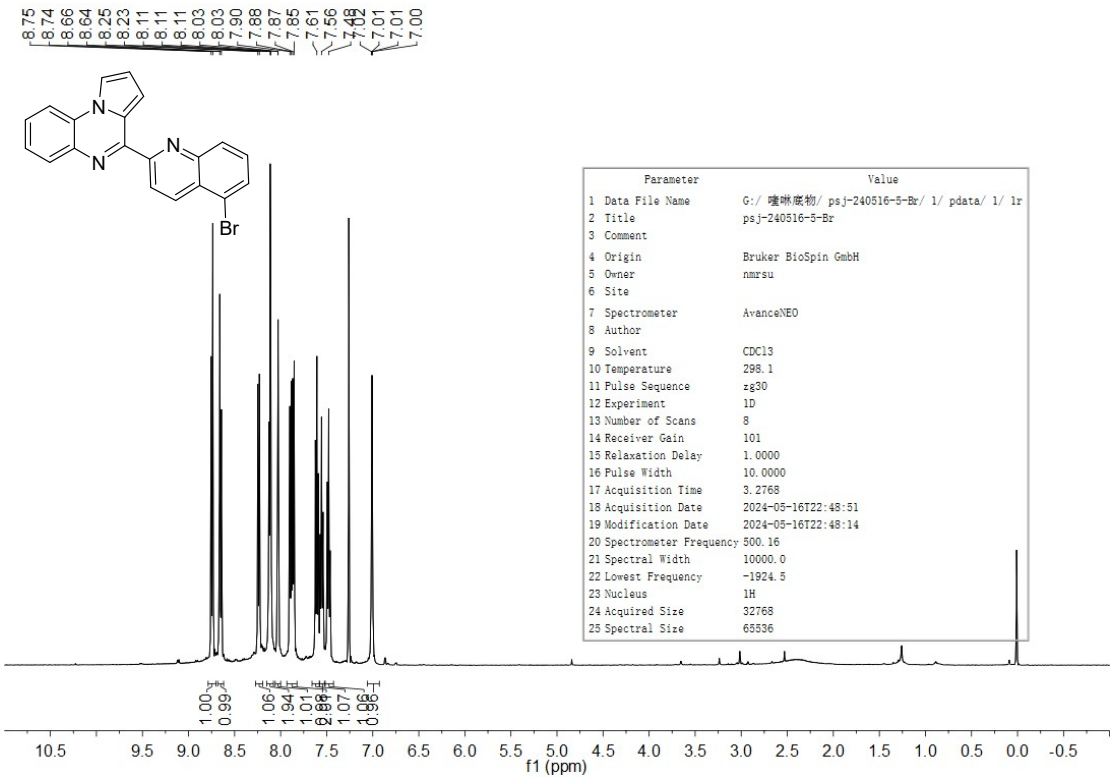


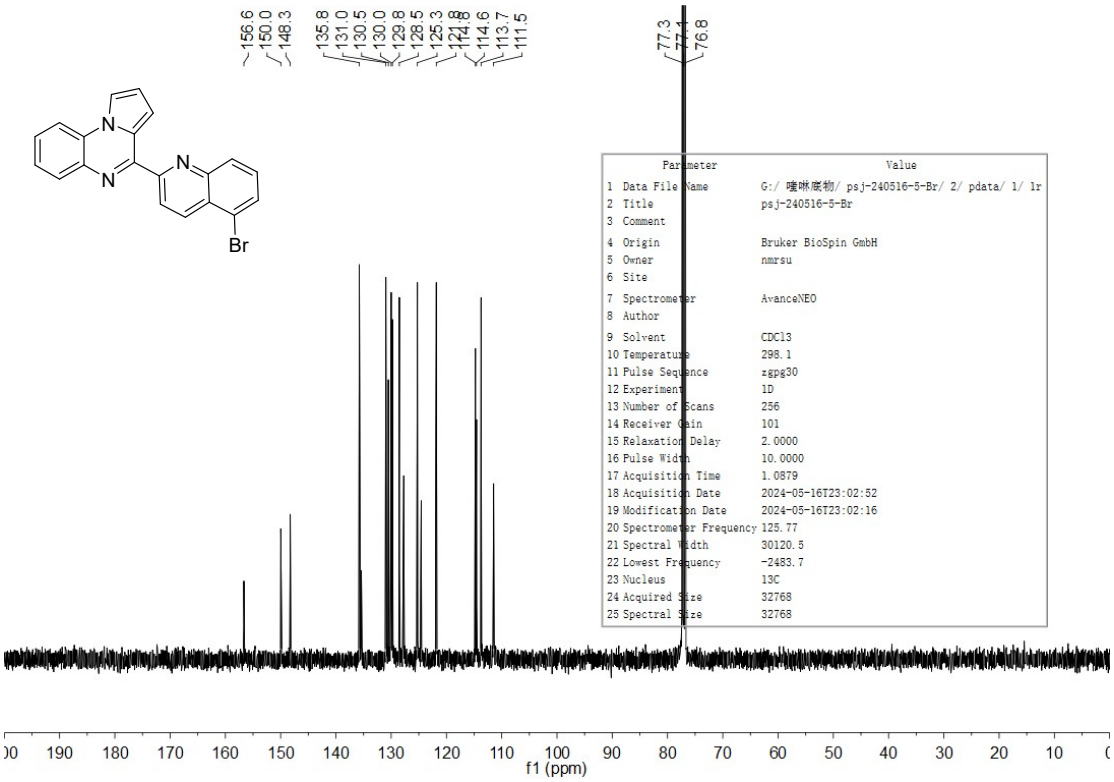
4-(8-methoxyquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ha)



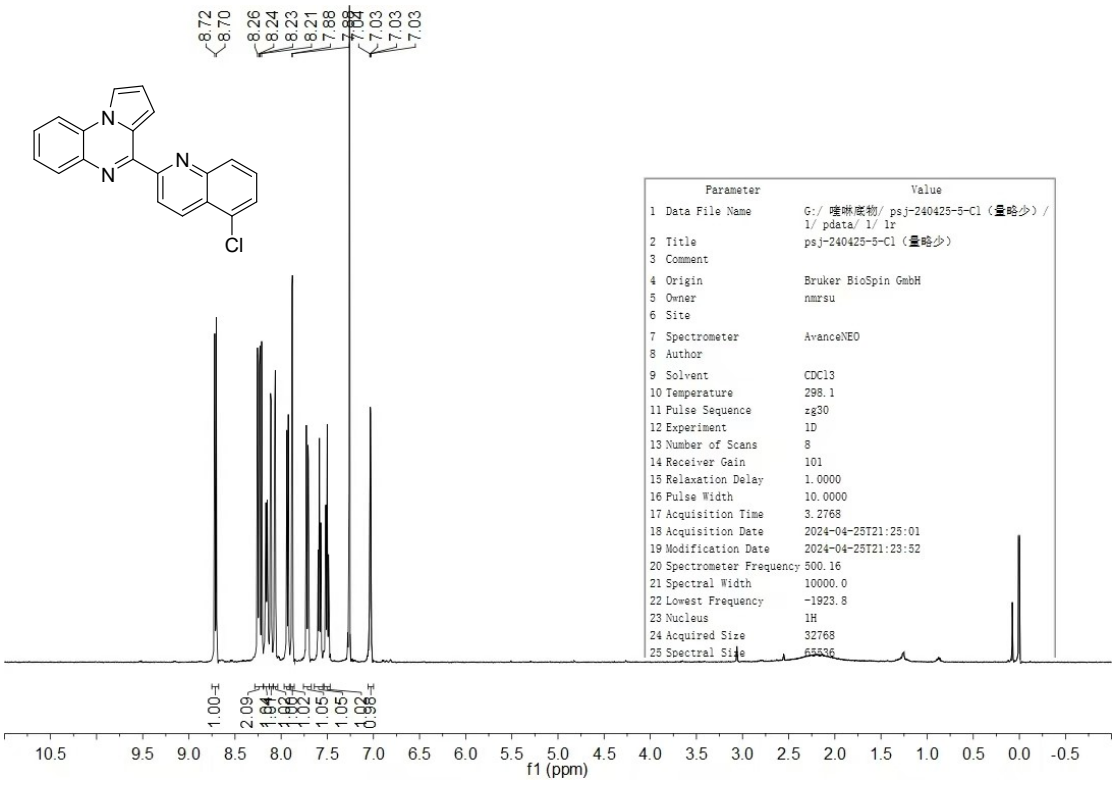


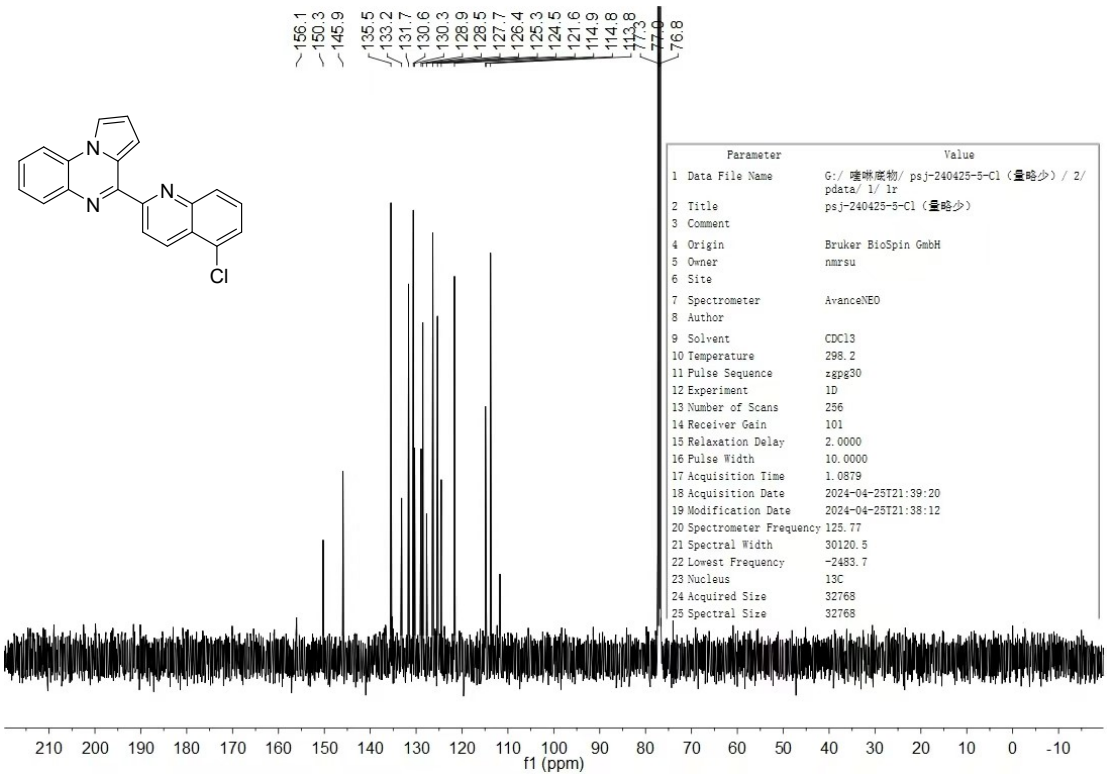
4-(5-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ia)



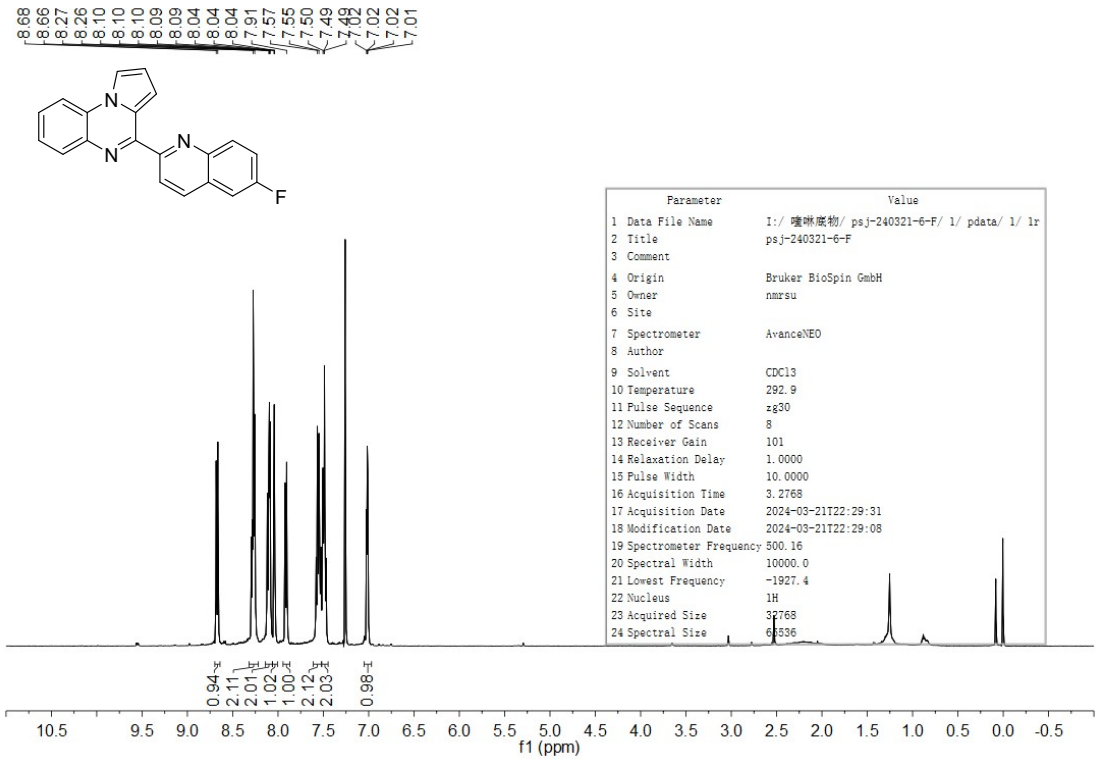


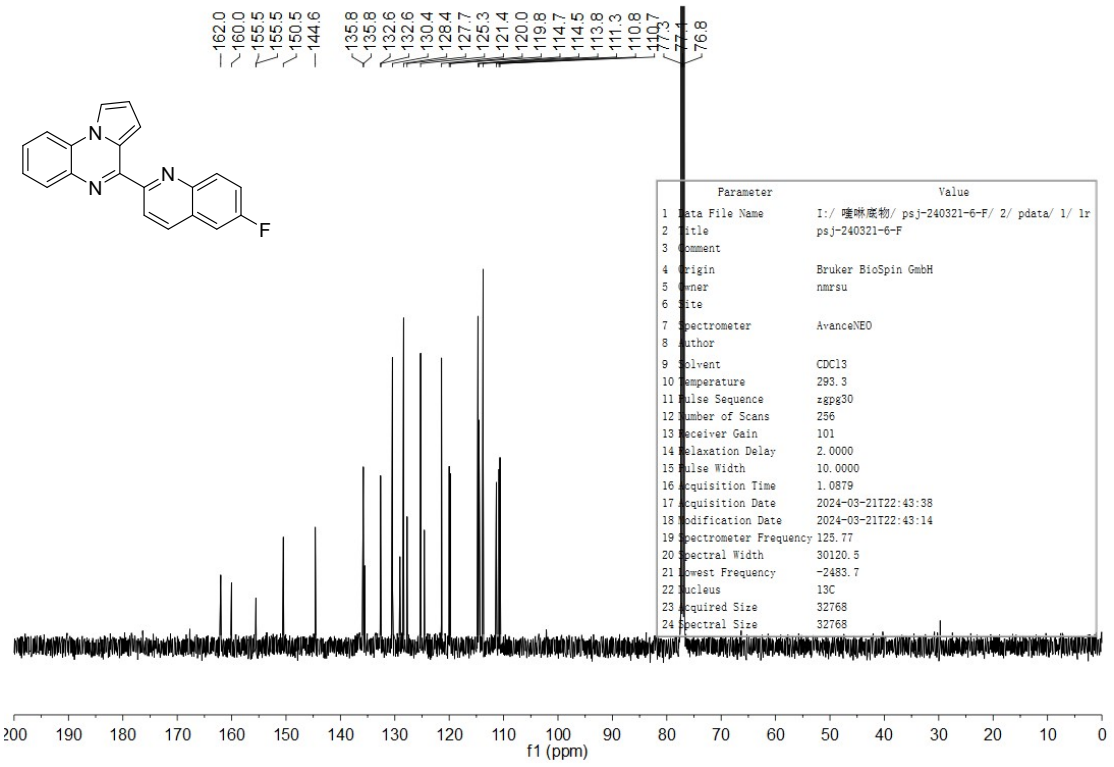
4-(5-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ja)



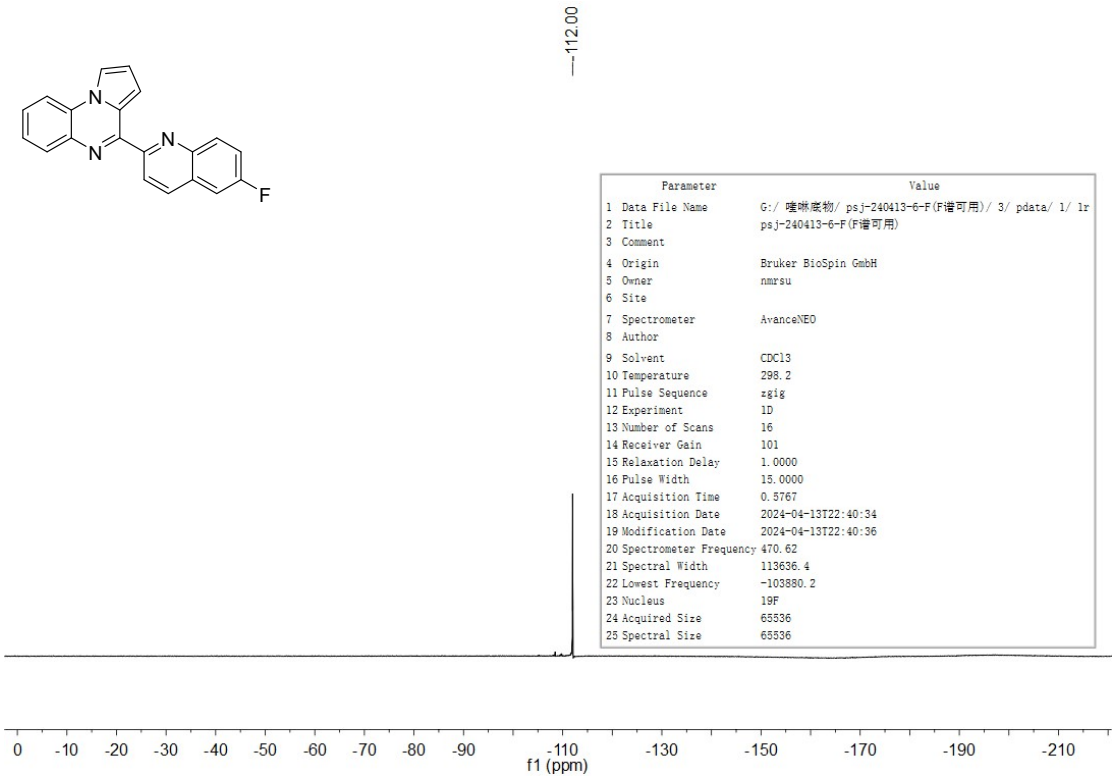


4-(6-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ka)[S5]



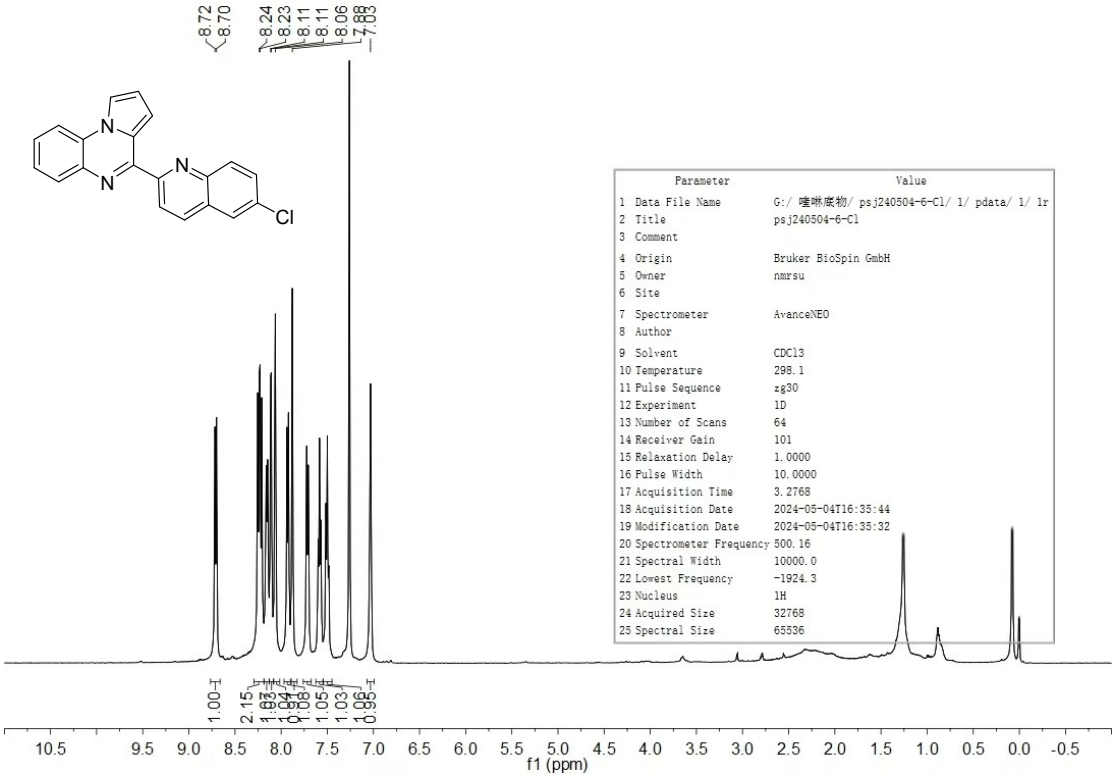


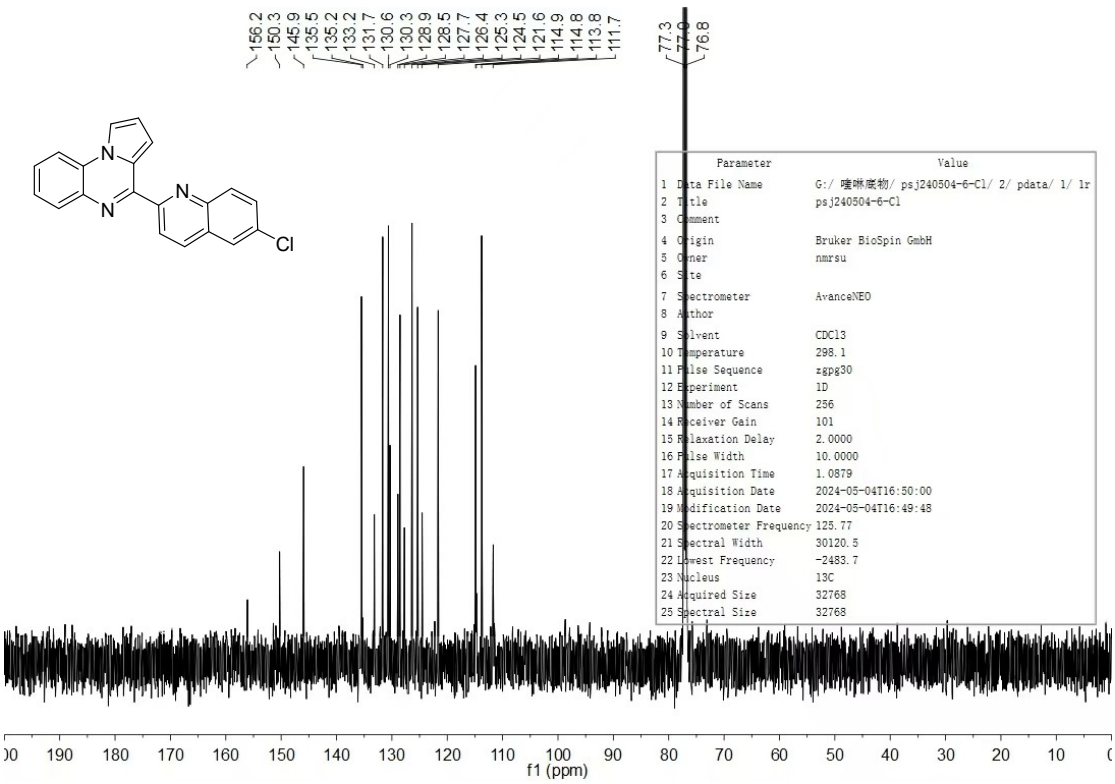
Parameter	Value
1 Data File Name	I:/ 喹啉底物/ psj-240321-6-F/ 2/ pdata/ 1/ 1r
2 Title	psj-240321-6-F
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	293.3
11 Pulse Sequence	zgpg30
12 Number of Scans	256
13 Receiver Gain	101
14 Relaxation Delay	2.0000
15 Pulse Width	10.0000
16 Acquisition Time	1.0879
17 Acquisition Date	2024-03-21T22:43:38
18 Modification Date	2024-03-21T22:43:14
19 Spectrometer Frequency	125.77
20 Spectral Width	30120.5
21 Lowest Frequency	-2483.7
22 Nucleus	13C
23 Acquired Size	32768
24 Spectral Size	32768



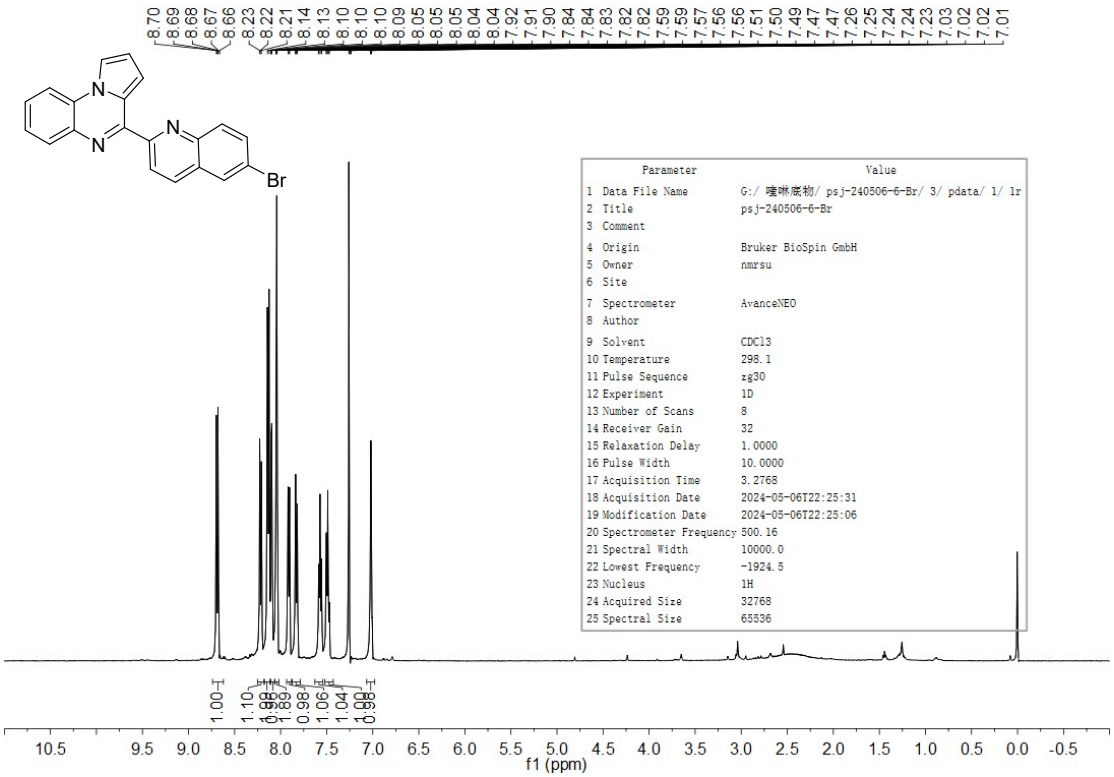
Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240413-6-F(F谱可用)/ 3/ pdata/ 1/ 1r
2 Title	psj-240413-6-F(F谱可用)
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-04-13T22:40:34
19 Modification Date	2024-04-13T22:40:36
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

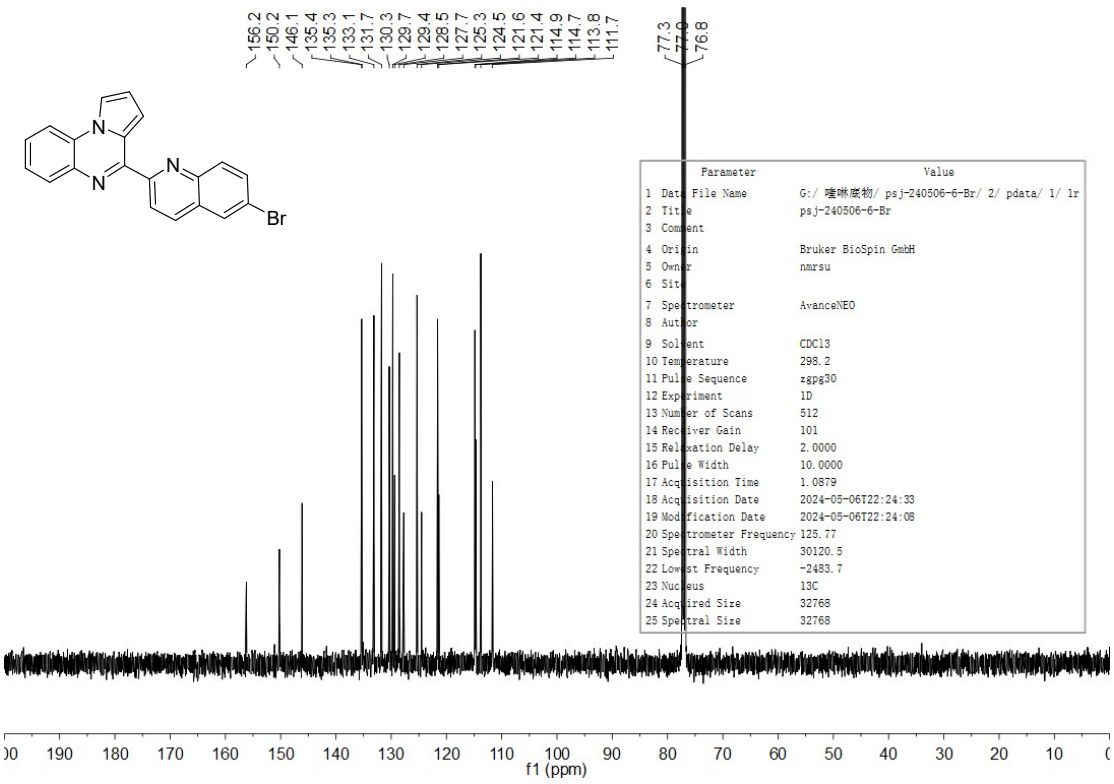
4-(6-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3la)



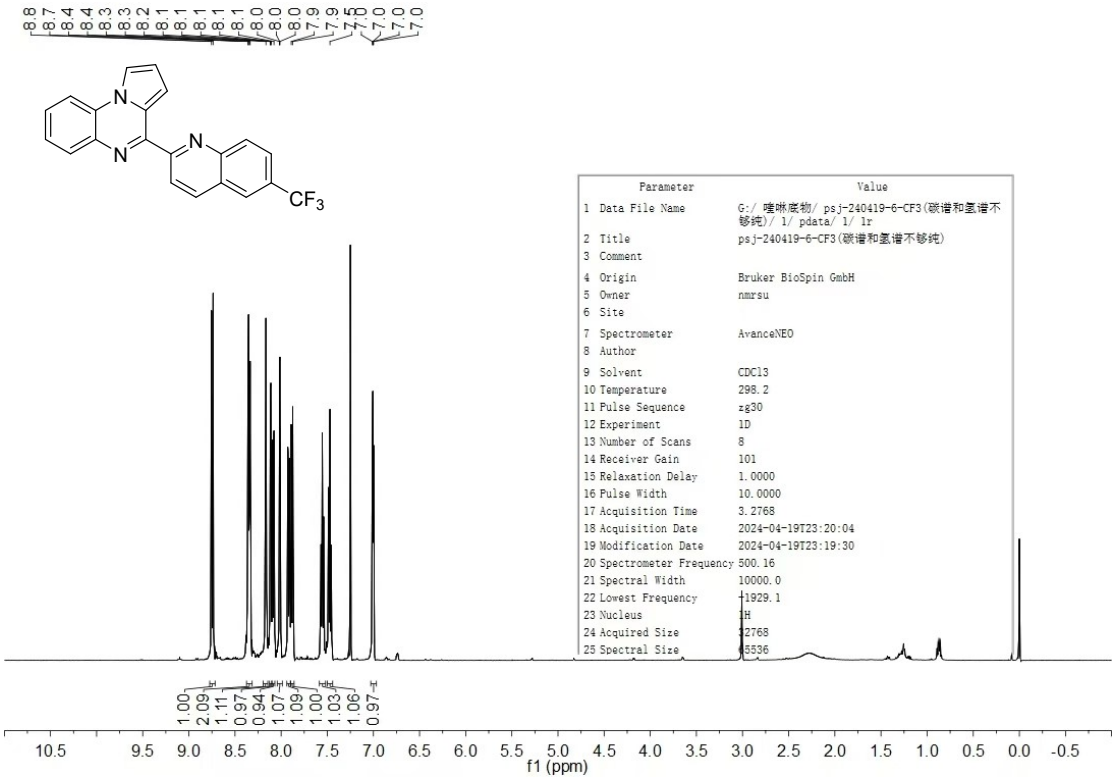


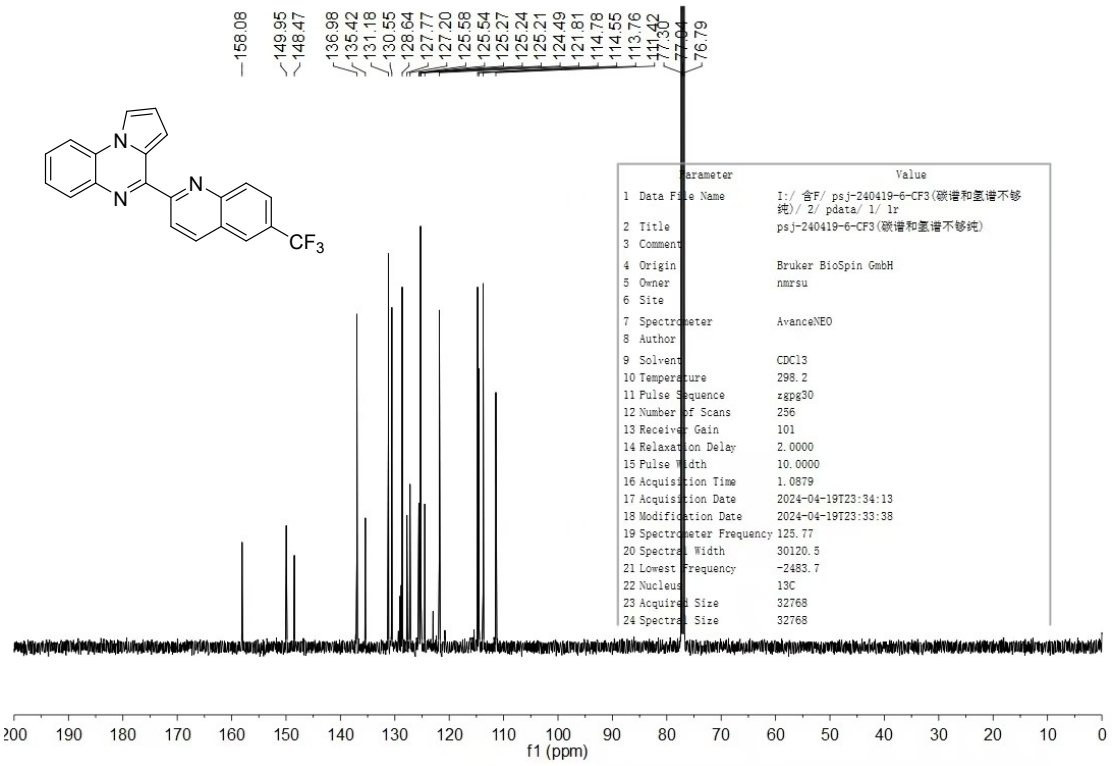
4-(6-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ma)

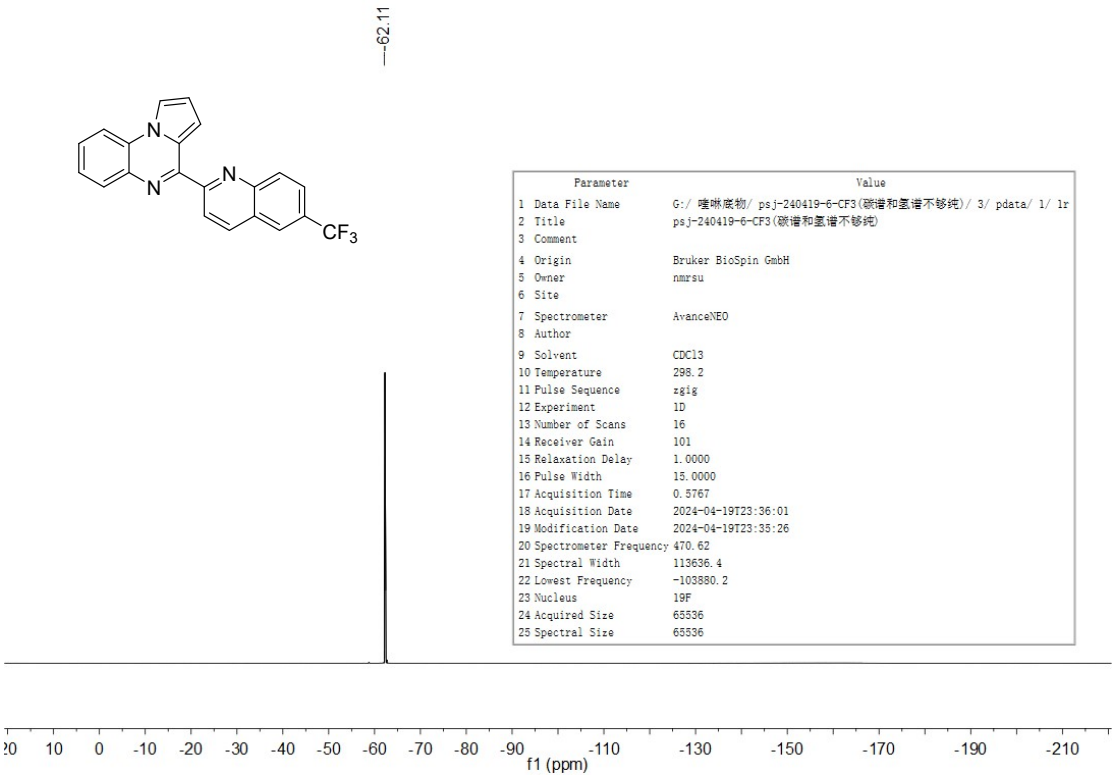




4-(6-(trifluoromethyl)quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3na)

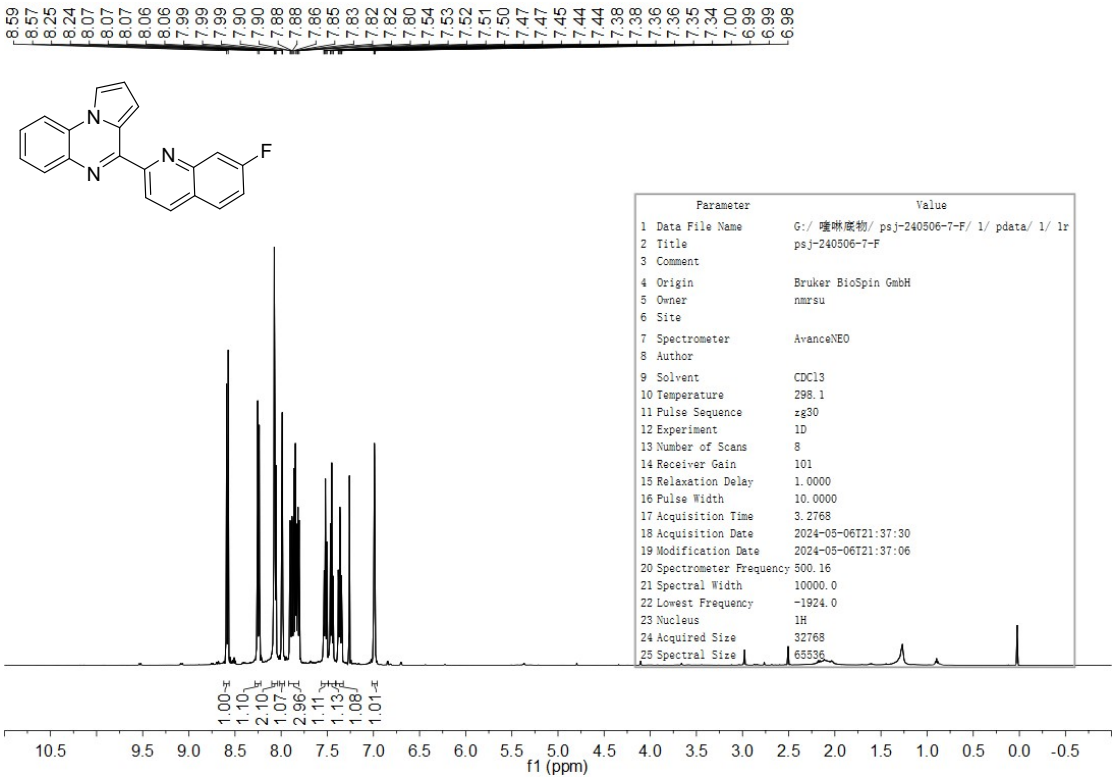




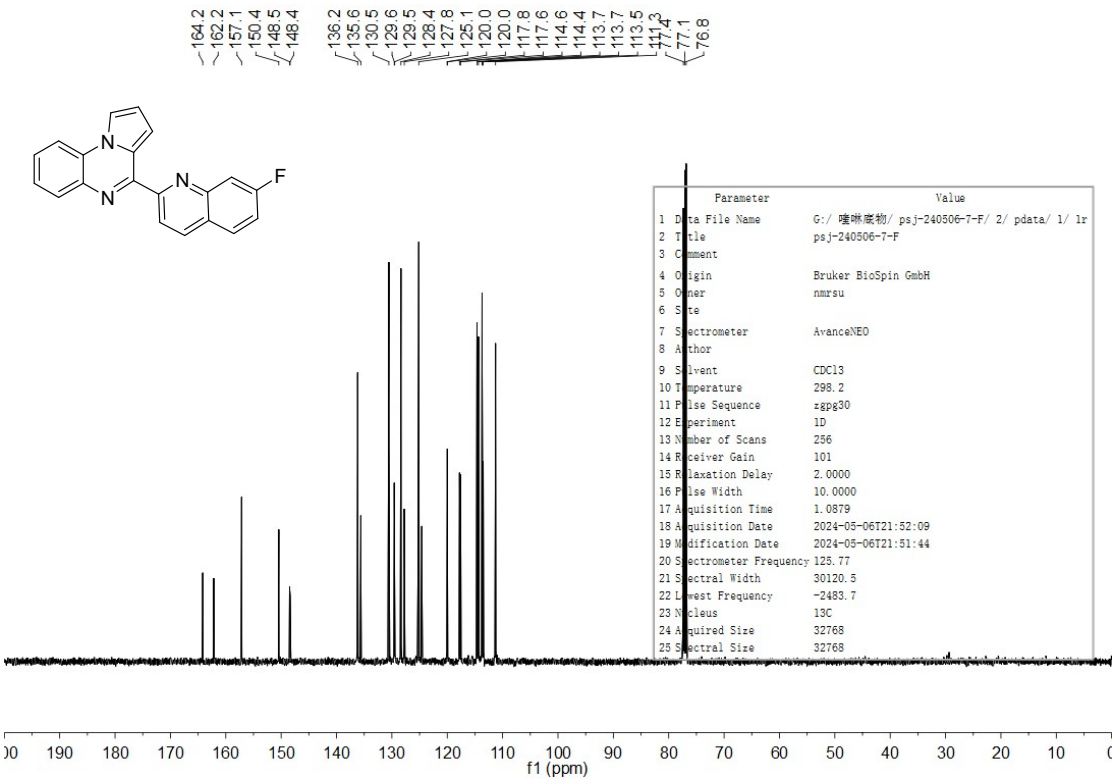


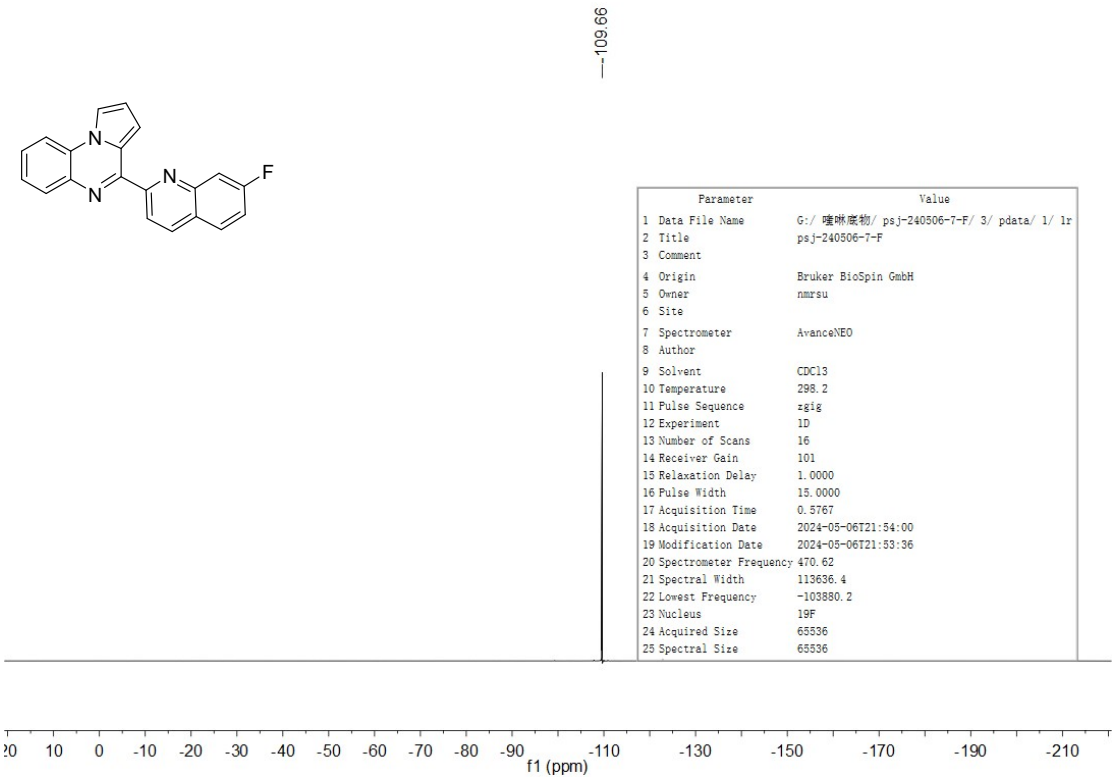
Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240419-6-CF3(碳谱和氢谱不够纯)/ 3/ pdata/ 1/ 1r
2 Title	psj-240419-6-CF3(碳谱和氢谱不够纯)
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-04-19T23:36:01
19 Modification Date	2024-04-19T23:35:26
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

4-(7-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3oa)[S3]

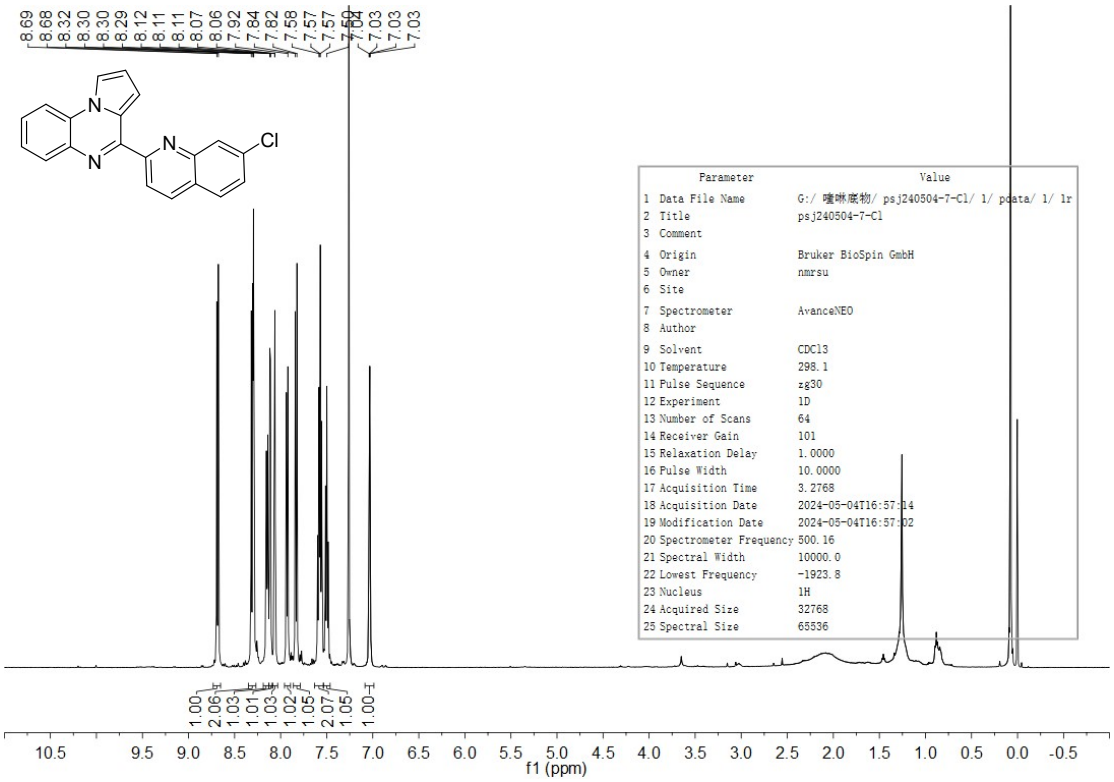


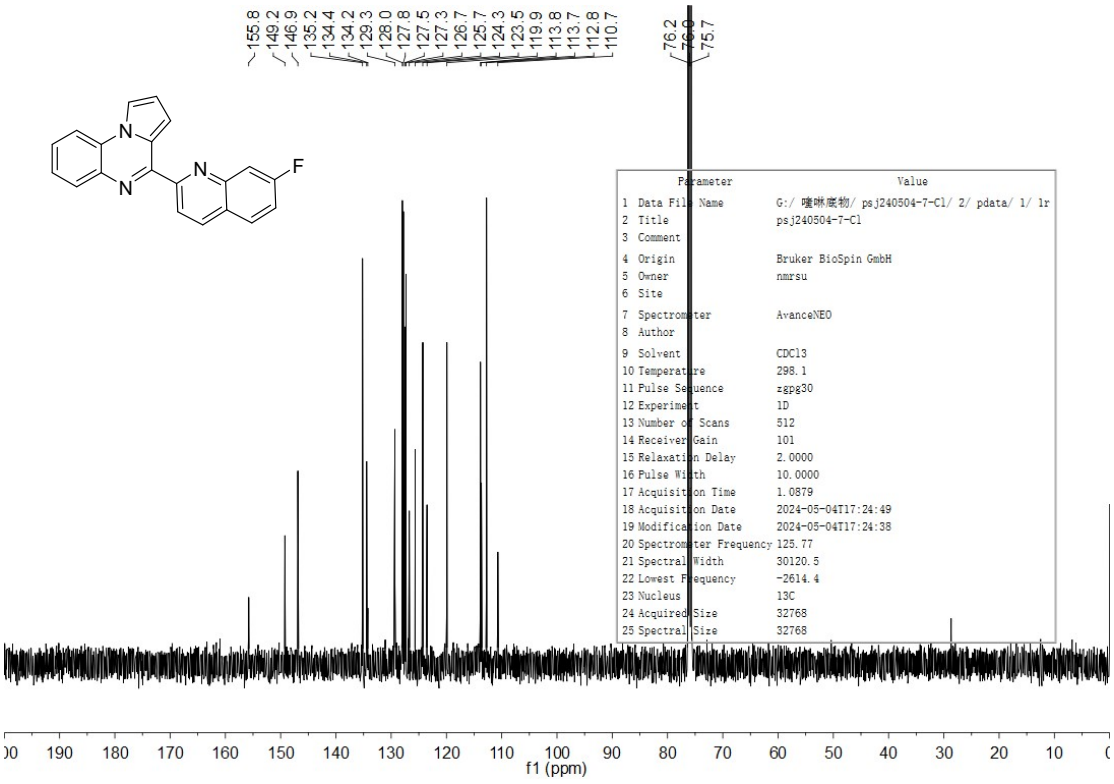
Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240506-7-F/ 1/ pdata/ 1/ 1r
2 Title	psj-240506-7-F
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-05-06T21:37:30
19 Modification Date	2024-05-06T21:37:06
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536


164.2
162.2
157.1
150.4
148.5
148.4
136.2
135.6
130.5
129.6
129.5
128.4
127.8
125.1
120.0
120.0
117.8
117.6
114.6
114.4
113.7
113.7
113.5
111.3
77.4
77.1
76.8
N
N
N
F
Parameter Value
1 Data File Name G:/ 喹啉底物/ psj-240506-7-F/ 2/ pdata/ 1/ 1r
2 Title psj-240506-7-F
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-05-06T21:52:09
19 Modification Date 2024-05-06T21:51:44
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

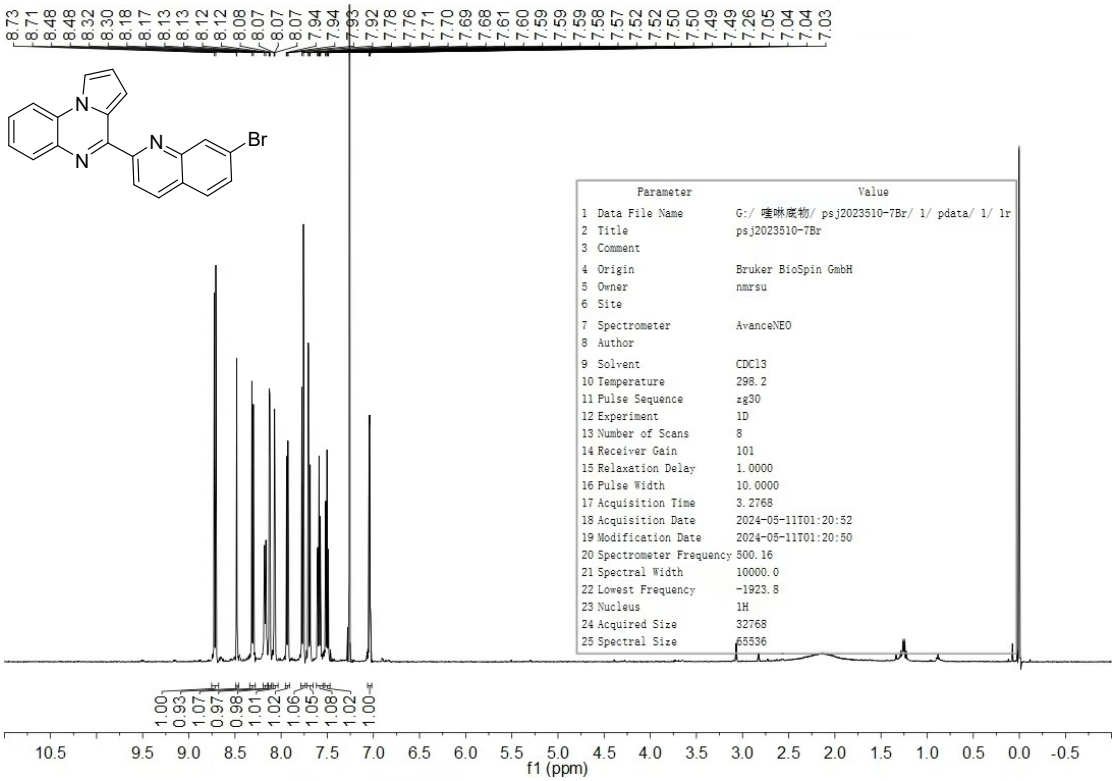

-109.66
N
N
N
F
Parameter Value
1 Data File Name G:/ 喹啉底物/ psj-240506-7-F/ 3/ pdata/ 1/ 1r
2 Title psj-240506-7-F
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgig
12 Experiment 1D
13 Number of Scans 16
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 15.0000
17 Acquisition Time 0.5767
18 Acquisition Date 2024-05-06T21:54:00
19 Modification Date 2024-05-06T21:53:36
20 Spectrometer Frequency 470.62
21 Spectral Width 113636.4
22 Lowest Frequency -103880.2
23 Nucleus 19F
24 Acquired Size 65536
25 Spectral Size 65536
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

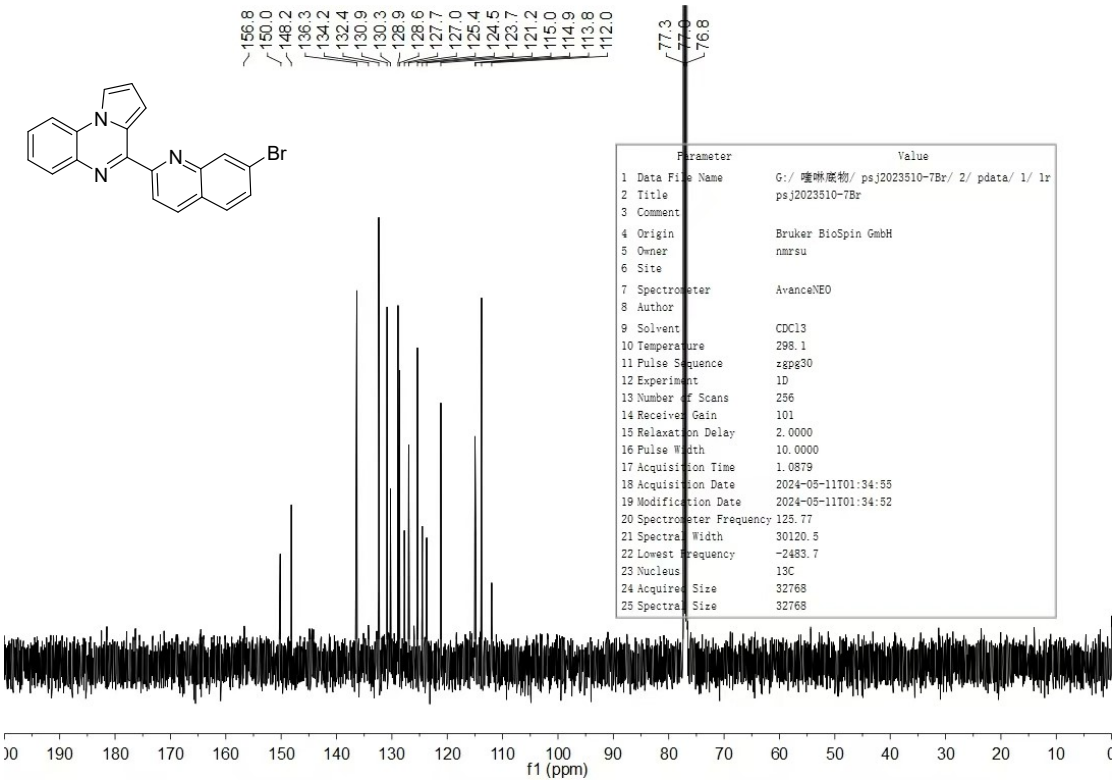
4-(7-chloroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3pa)



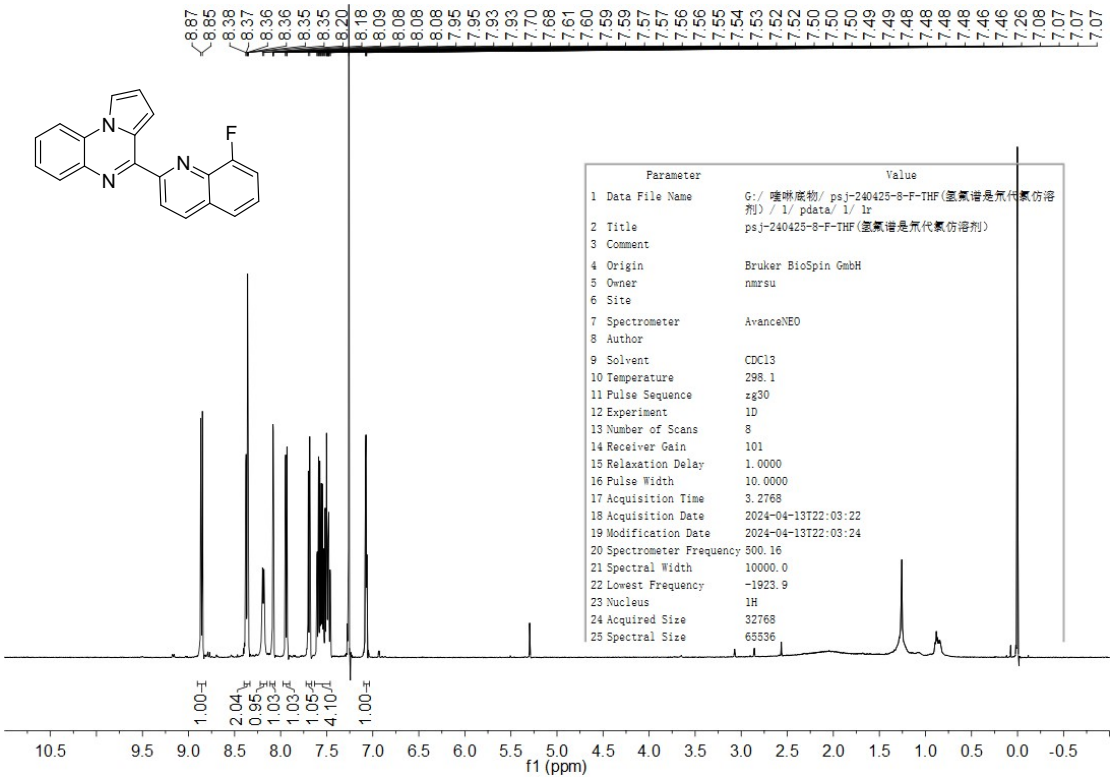


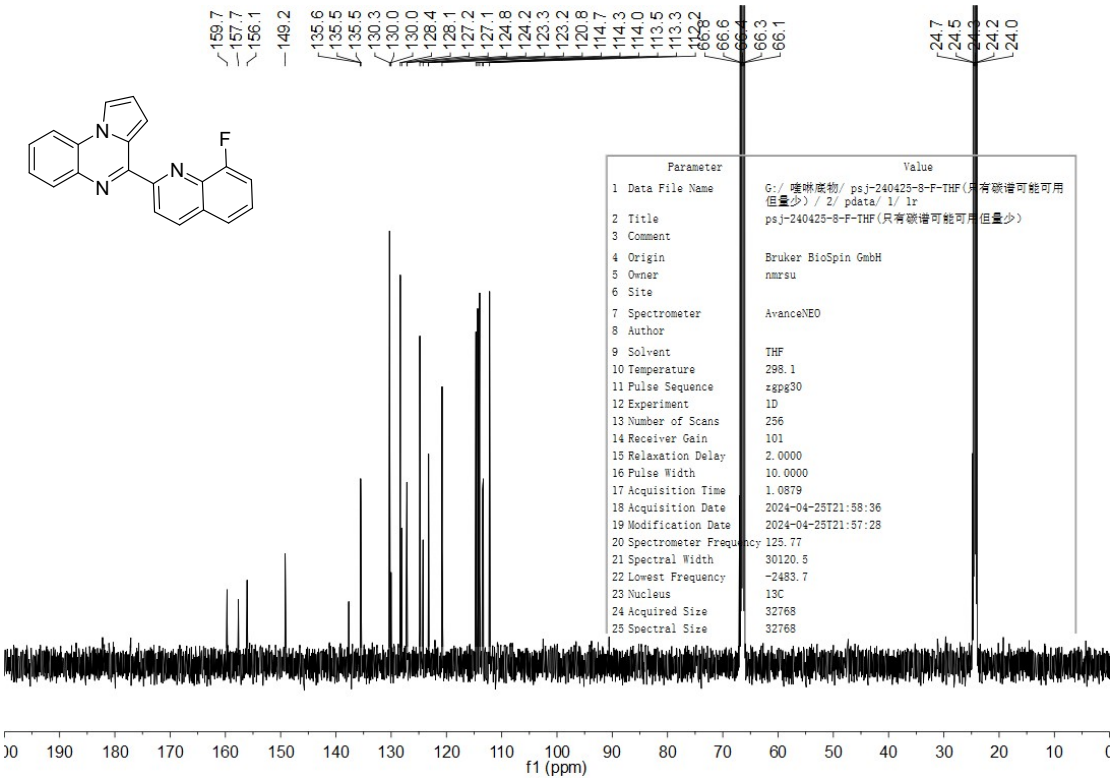
4-(7-bromoquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3qa)

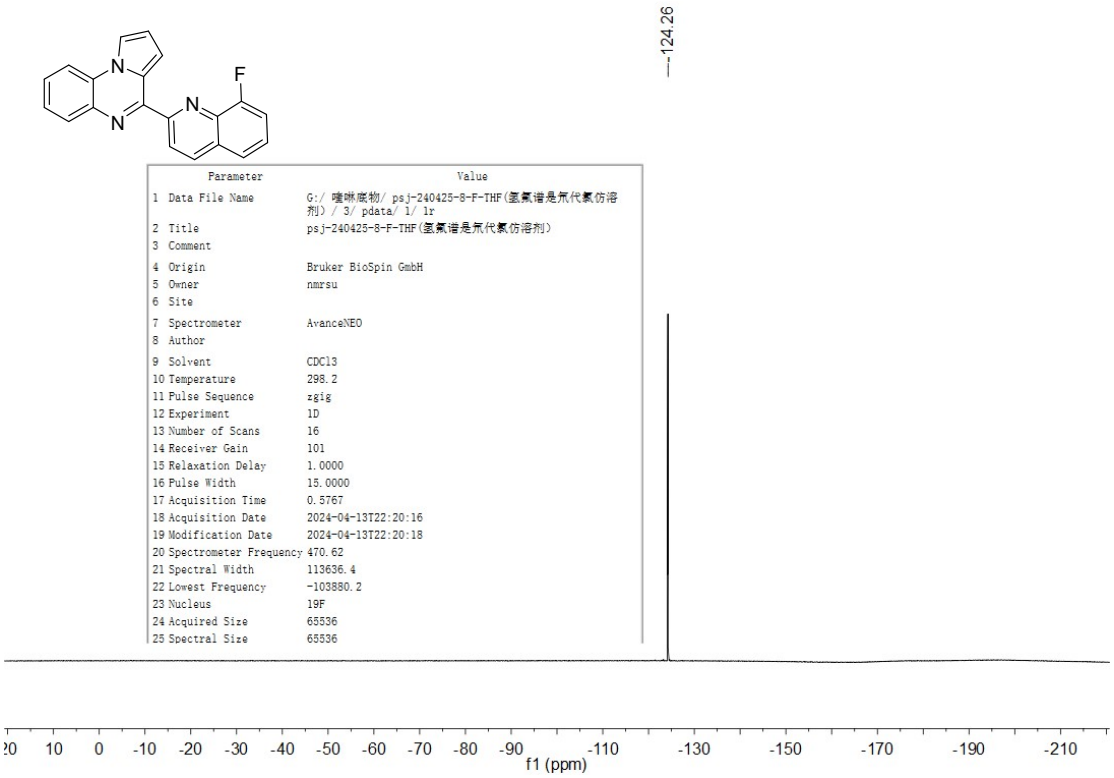




4-(8-fluoroquinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ra)

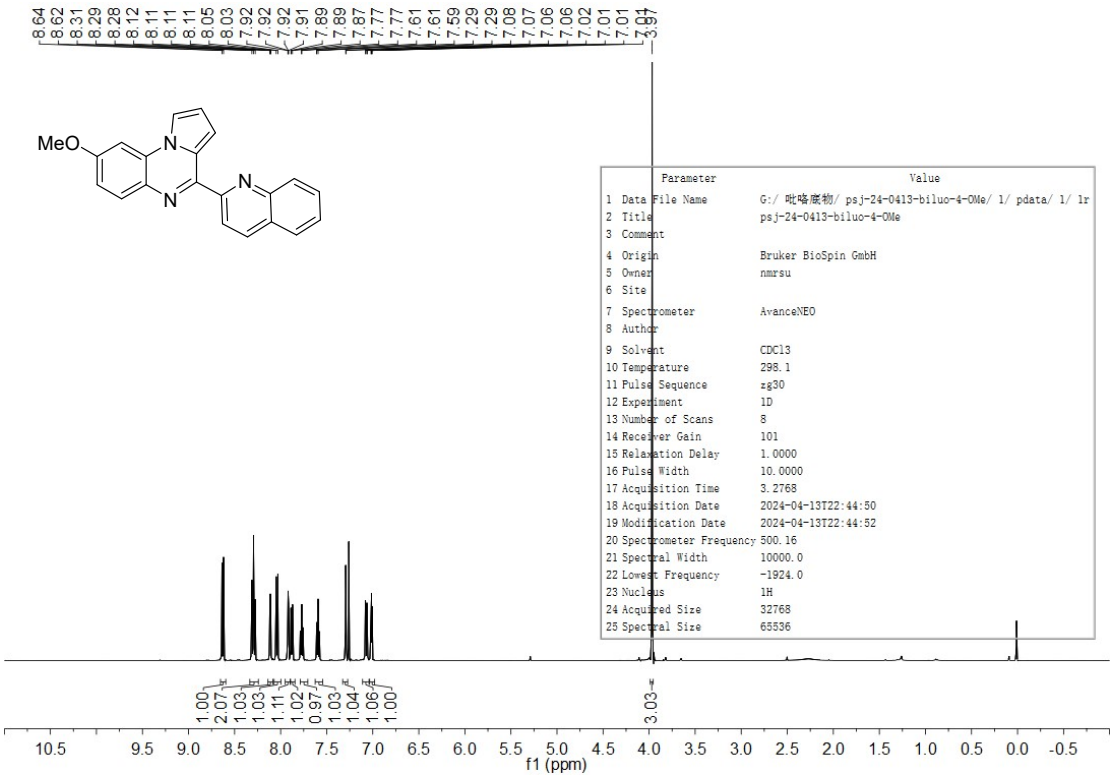




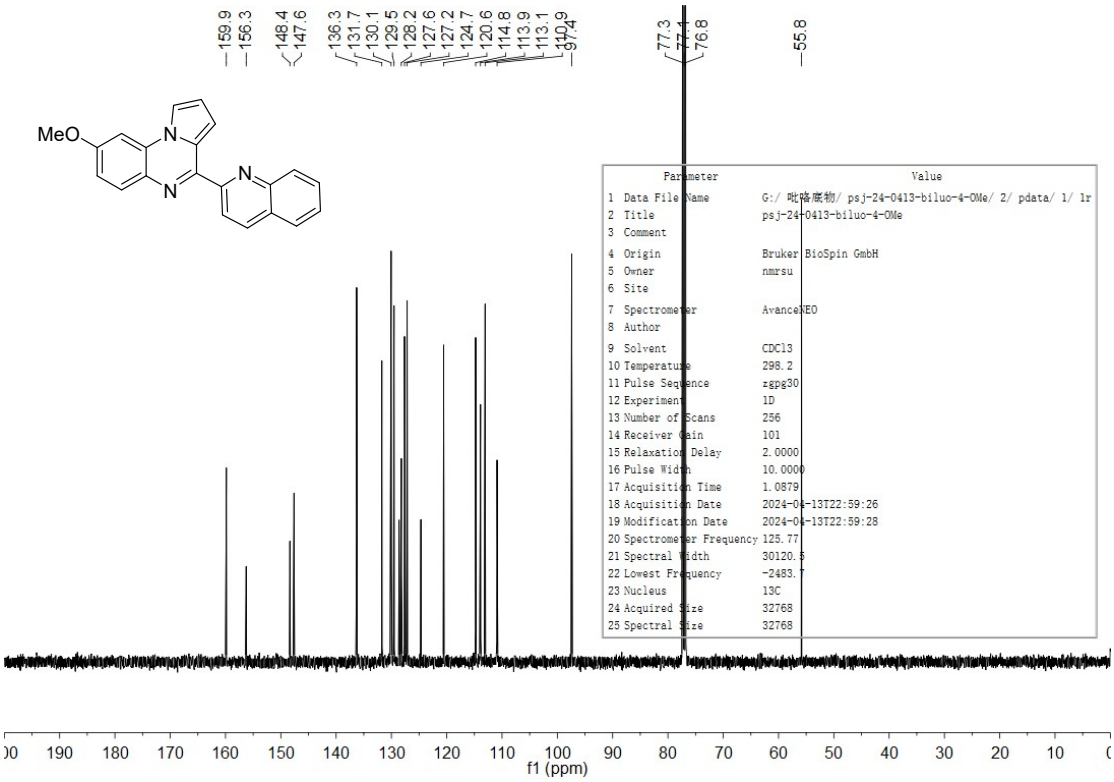


Parameter	Value
1 Data File Name	G:/ 喹啉底物/ psj-240425-8-F-THF(氢氟谱是氘代氯仿溶剂) / 3/ pdata/ 1/ 1r
2 Title	psj-240425-8-F-THF(氢氟谱是氘代氯仿溶剂)
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-04-13T22:20:16
19 Modification Date	2024-04-13T22:20:18
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

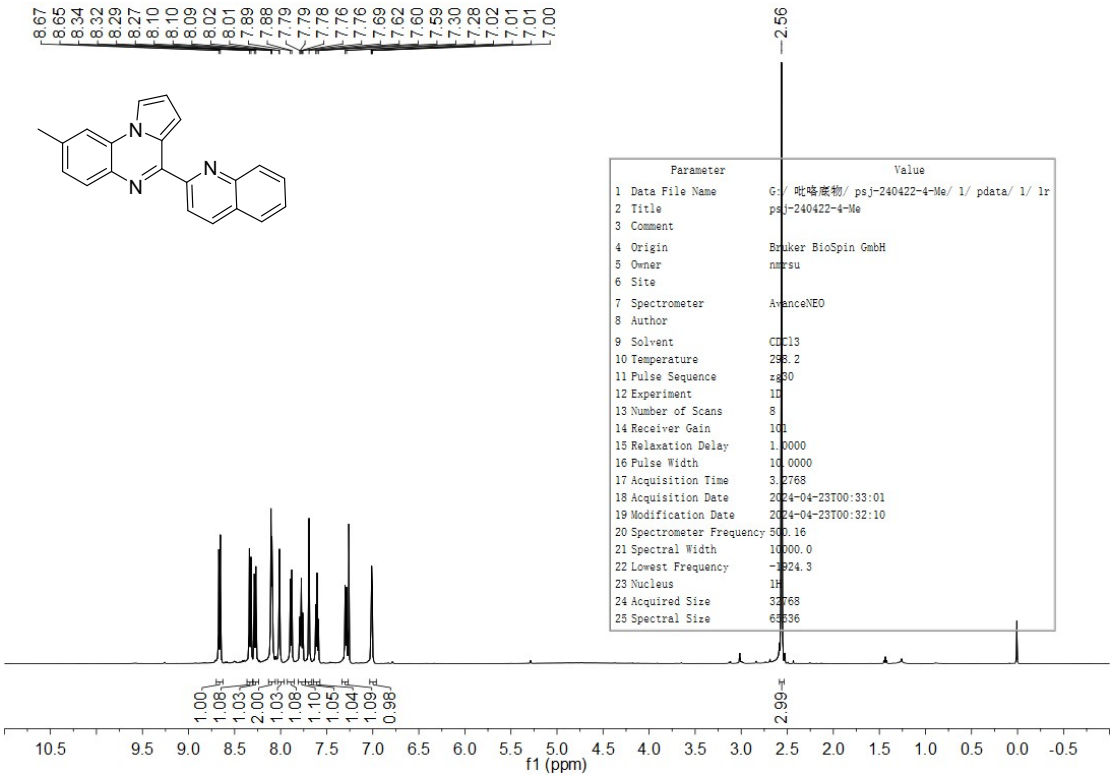
8-methoxy-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ab)[S4]

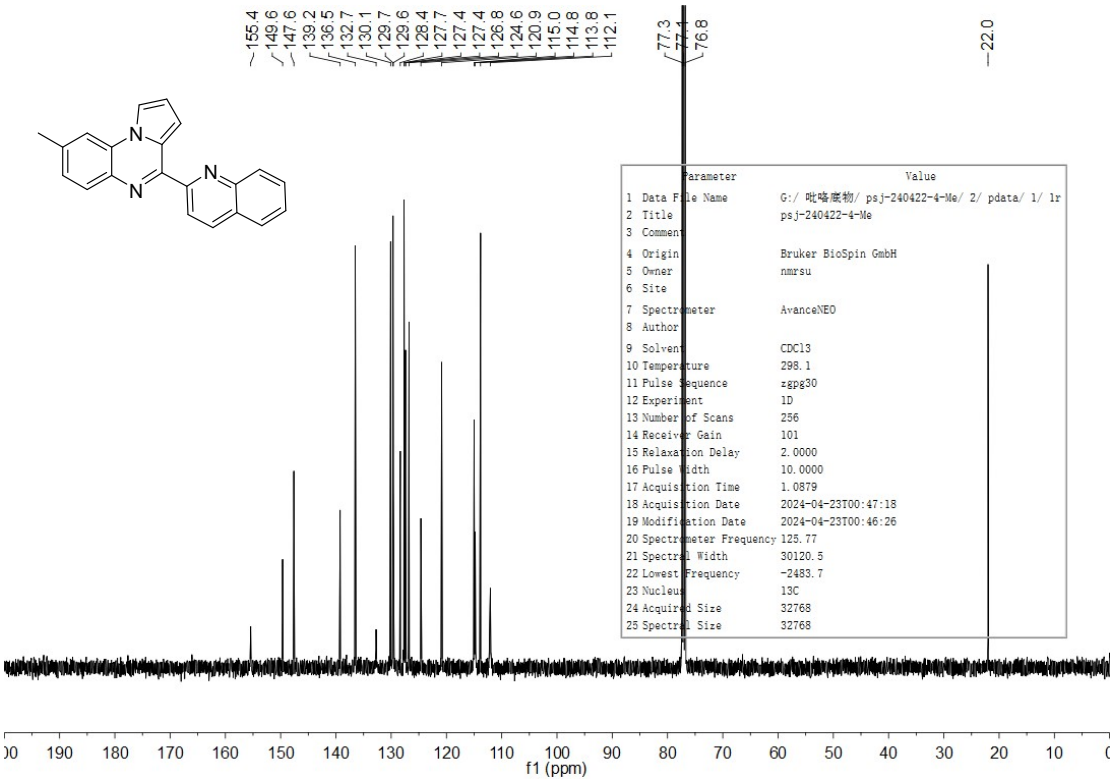


Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj-24-0413-biluo-4-OMe/ 1/ pdata/ 1/ 1r
2 Title	psj-24-0413-biluo-4-OMe
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-04-13T22:44:50
19 Modification Date	2024-04-13T22:44:52
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536



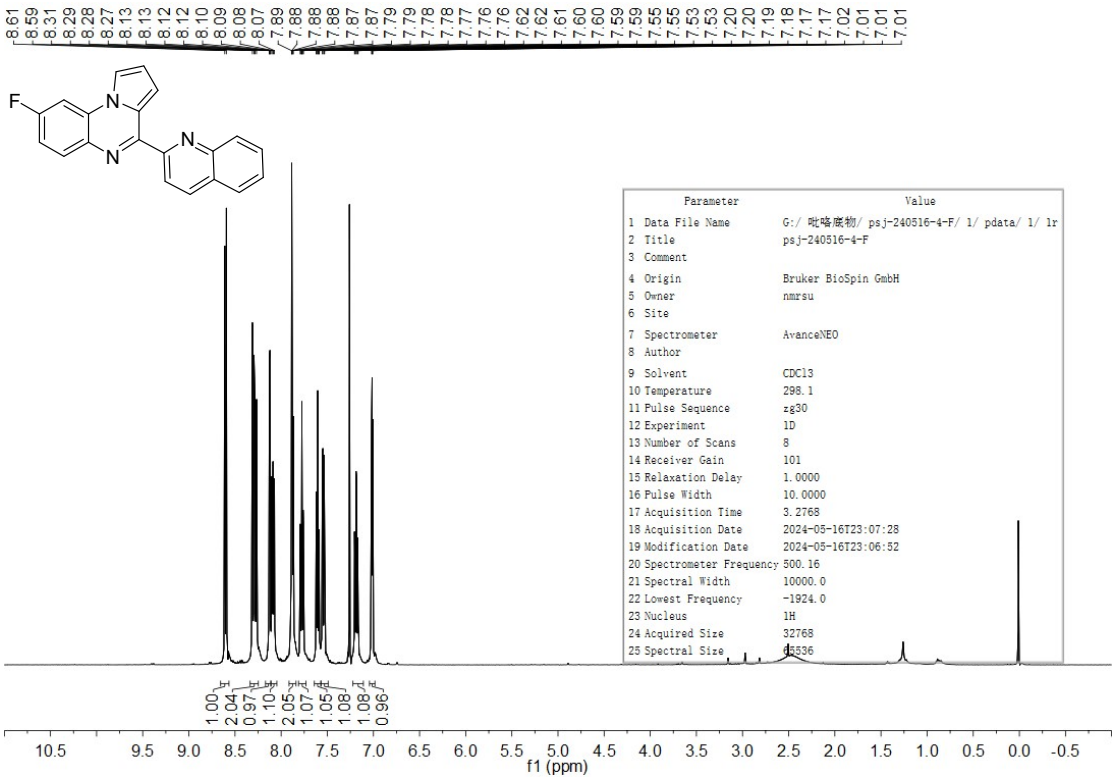
8-methyl-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ac)



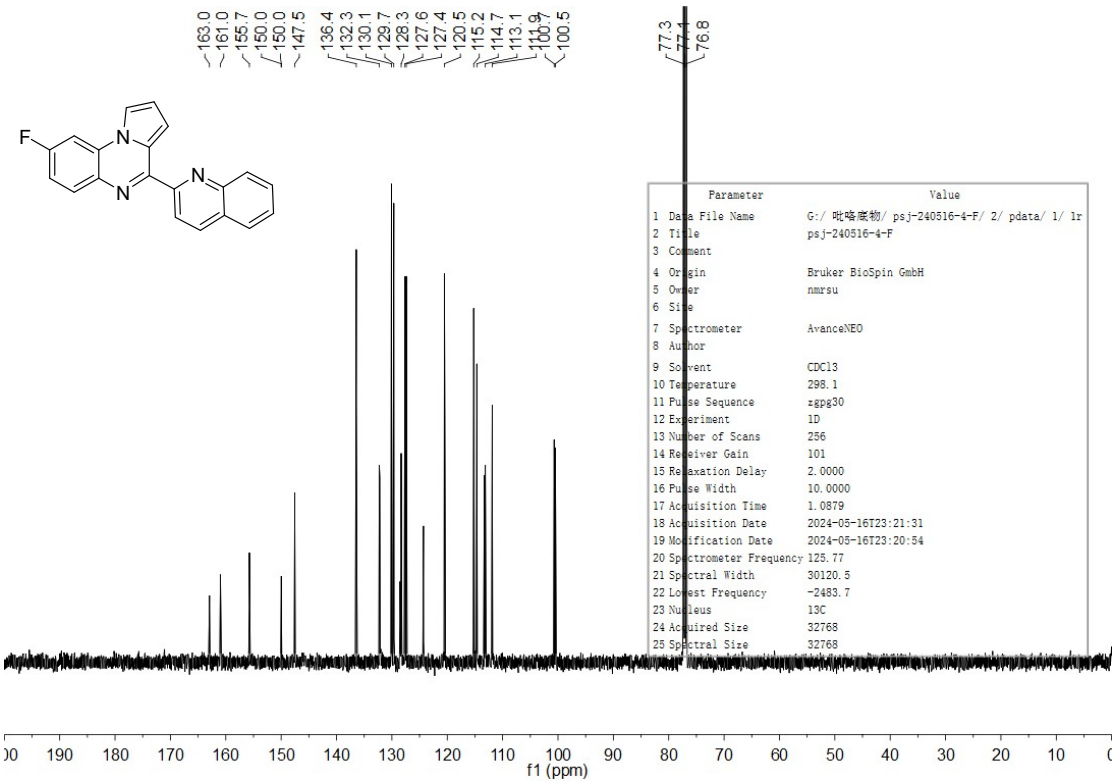


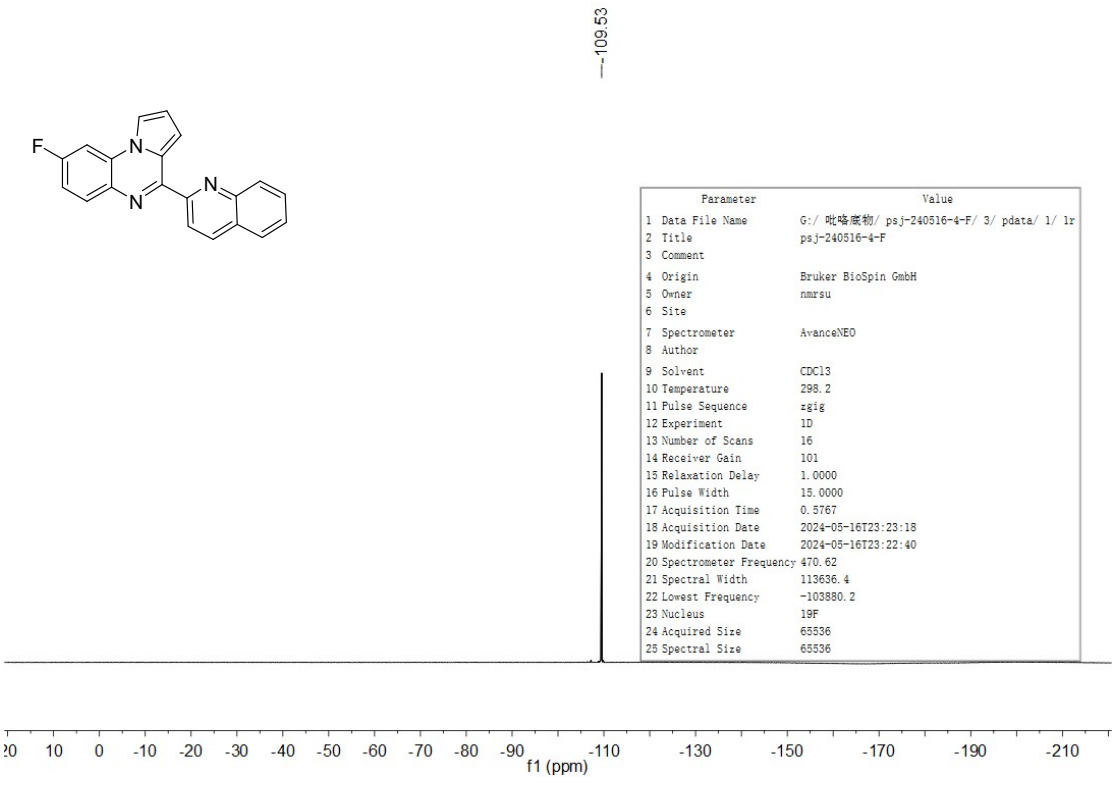
	Parameter	Value
1	Data File Name	G:/ 吡咯底物/ psj-240422-4-Me/ 2/ pdata/ 1/ 1r
2	Title	psj-240422-4-Me
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zgpg30
12	Experiment	1D
13	Number of Scans	256
14	Receiver Gain	101
15	Relaxation Delay	2.0000
16	Pulse Width	10.0000
17	Acquisition Time	1.0879
18	Acquisition Date	2024-04-23T00:47:18
19	Modification Date	2024-04-23T00:46:26
20	Spectrometer Frequency	125.77
21	Spectral Width	30120.5
22	Lowest Frequency	-2483.7
23	Nucleus	13C
24	Acquired Size	32768
25	Spectral Size	32768

8-fluoro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ad)[S4]

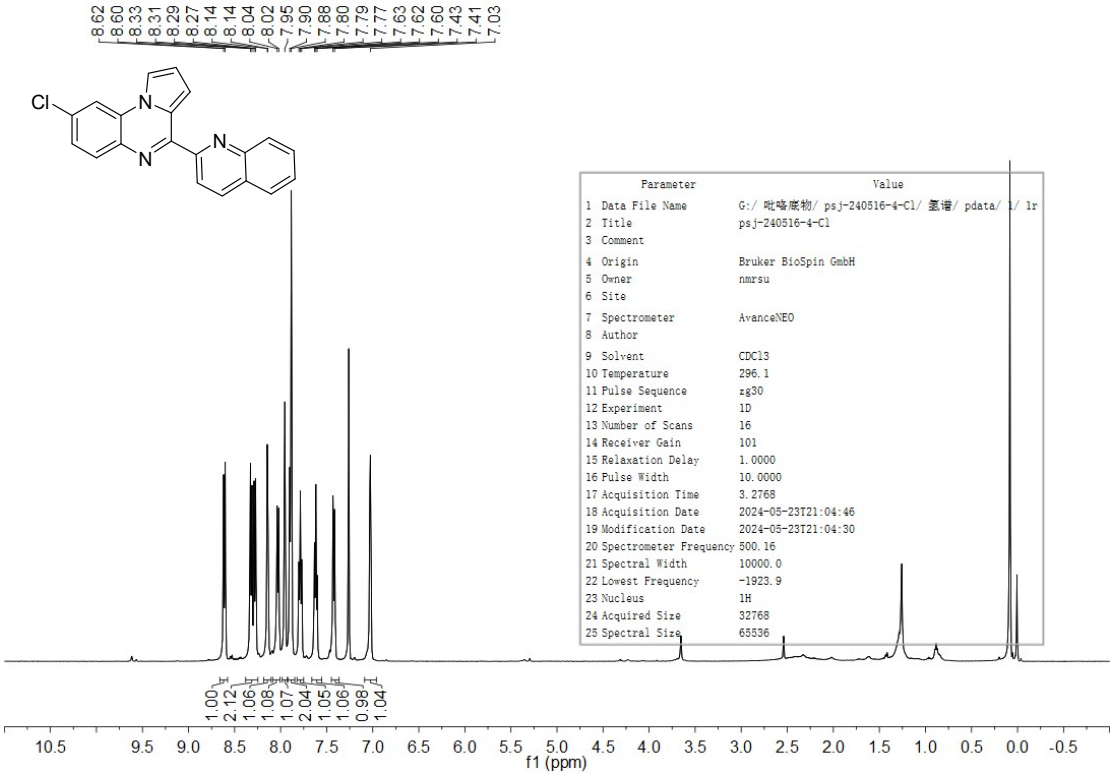


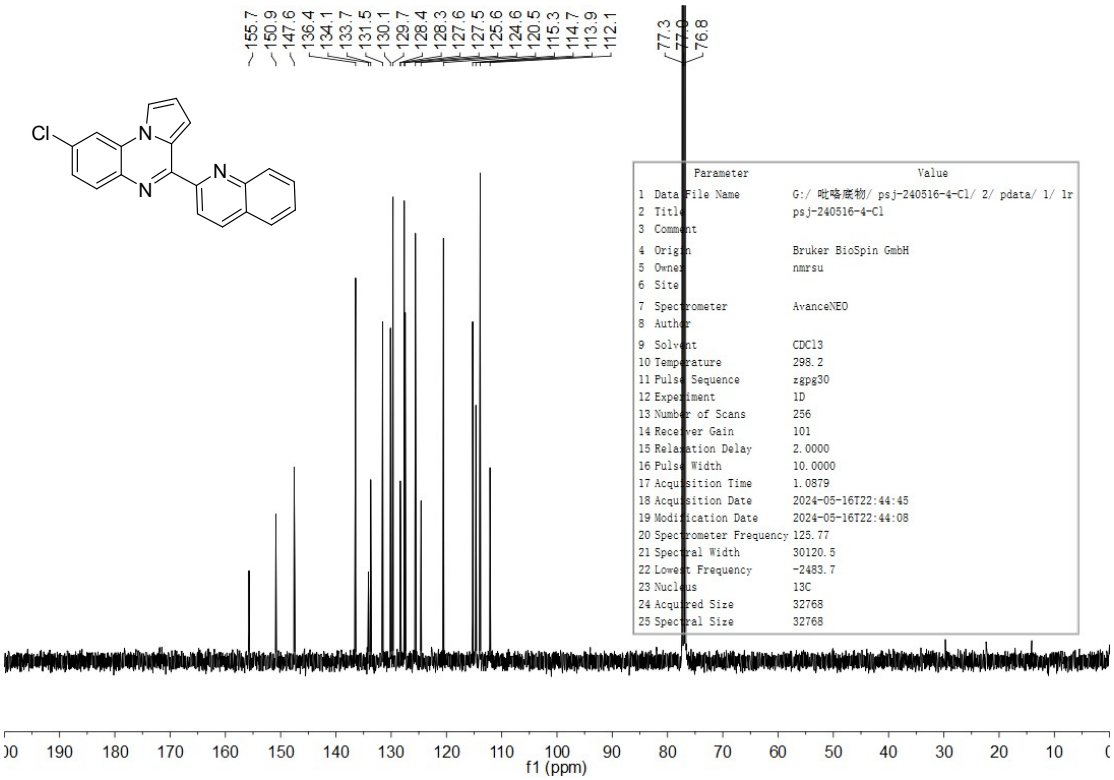
	Parameter	Value
1	Data File Name	G:/ 吡咯底物/ psj-240516-4-F/ 1/ pdata/ 1/ 1r
2	Title	psj-240516-4-F
3	Comment	
4	Origin	Bruker BioSpin GmbH
5	Owner	nmrsu
6	Site	
7	Spectrometer	AvanceNEO
8	Author	
9	Solvent	CDCl3
10	Temperature	298.1
11	Pulse Sequence	zg30
12	Experiment	1D
13	Number of Scans	8
14	Receiver Gain	101
15	Relaxation Delay	1.0000
16	Pulse Width	10.0000
17	Acquisition Time	3.2768
18	Acquisition Date	2024-05-16T23:07:28
19	Modification Date	2024-05-16T23:06:52
20	Spectrometer Frequency	500.16
21	Spectral Width	10000.0
22	Lowest Frequency	-1924.0
23	Nucleus	1H
24	Acquired Size	32768
25	Spectral Size	65536


163.0
161.0
155.7
150.0
150.0
147.5
136.4
132.3
130.1
129.7
128.3
127.6
127.4
120.5
115.2
114.7
113.1
111.9
100.5
77.3
77.4
76.8
F
N
N
N
Parameter Value
1 Data File Name G:/ 吡咯底物/ psj-240516-4-F/ 2/ pdata/ 1/ 1r
2 Title psj-240516-4-F
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.1
11 Pulse Sequence zgpg30
12 Experiment 1D
13 Number of Scans 256
14 Receiver Gain 101
15 Relaxation Delay 2.0000
16 Pulse Width 10.0000
17 Acquisition Time 1.0879
18 Acquisition Date 2024-05-16T23:21:31
19 Modification Date 2024-05-16T23:20:54
20 Spectrometer Frequency 125.77
21 Spectral Width 30120.5
22 Lowest Frequency -2483.7
23 Nucleus 13C
24 Acquired Size 32768
25 Spectral Size 32768
190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10
f1 (ppm)

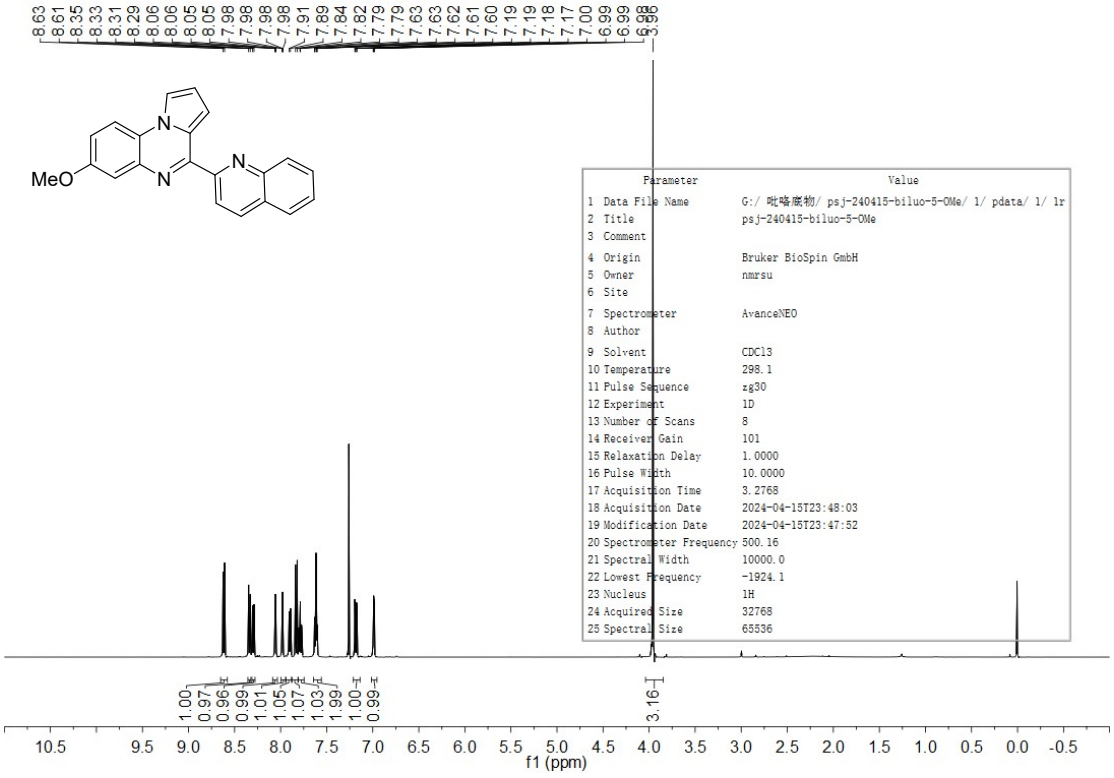

109.53
F
N
N
N
Parameter Value
1 Data File Name G:/ 吡咯底物/ psj-240516-4-F/ 3/ pdata/ 1/ 1r
2 Title psj-240516-4-F
3 Comment
4 Origin Bruker BioSpin GmbH
5 Owner nmrsu
6 Site
7 Spectrometer AvanceNEO
8 Author
9 Solvent CDCl3
10 Temperature 298.2
11 Pulse Sequence zgig
12 Experiment 1D
13 Number of Scans 16
14 Receiver Gain 101
15 Relaxation Delay 1.0000
16 Pulse Width 15.0000
17 Acquisition Time 0.5767
18 Acquisition Date 2024-05-16T23:23:18
19 Modification Date 2024-05-16T23:22:40
20 Spectrometer Frequency 470.62
21 Spectral Width 113636.4
22 Lowest Frequency -103880.2
23 Nucleus 19F
24 Acquired Size 65536
25 Spectral Size 65536
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -110 -130 -150 -170 -190 -210
f1 (ppm)

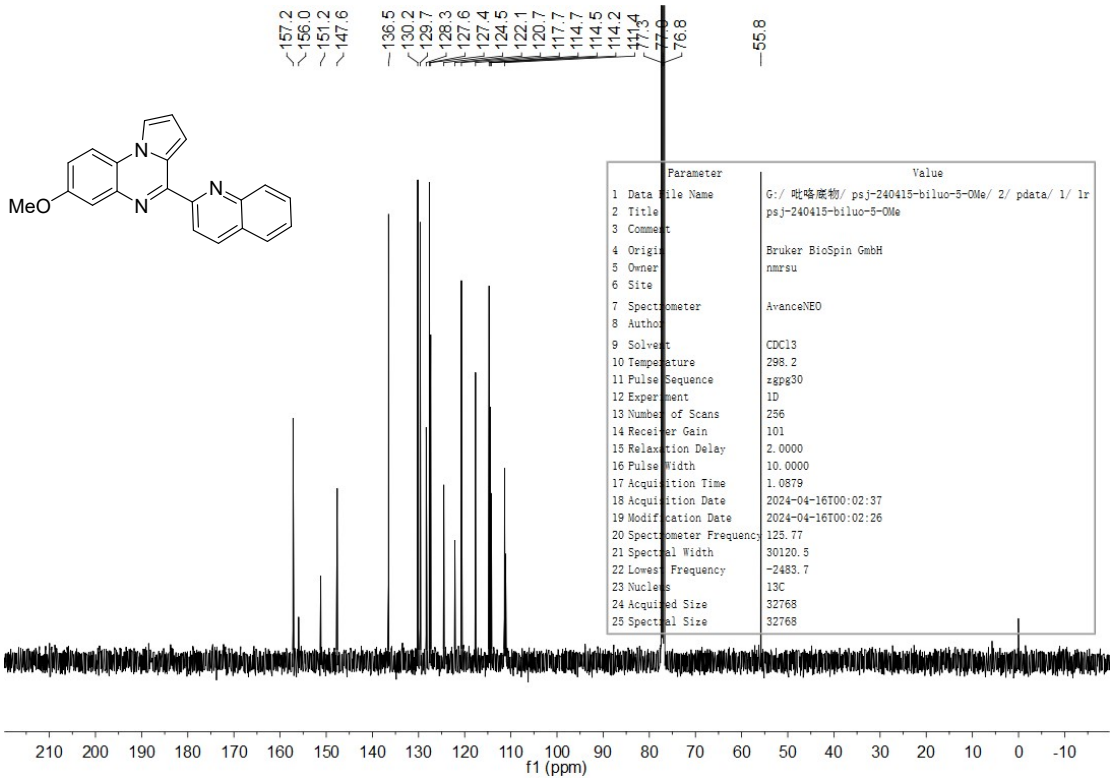
8-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ae)



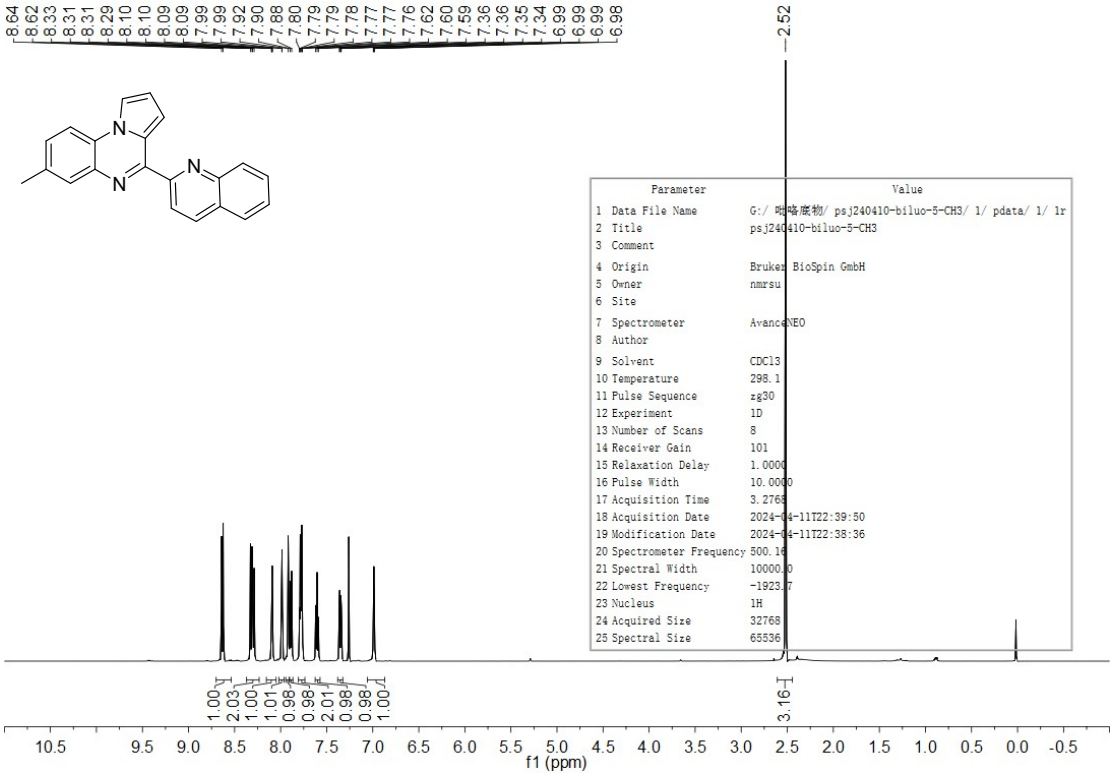


7-methoxy-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3af)

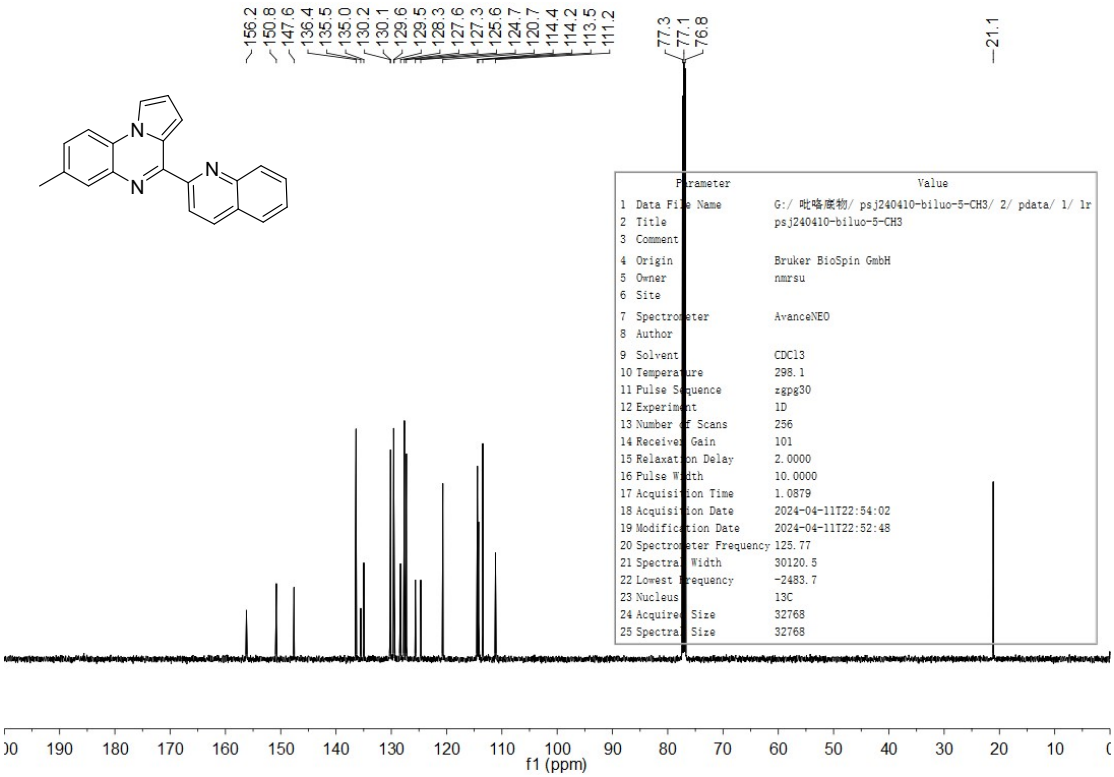




7-methyl-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ag)[S4]

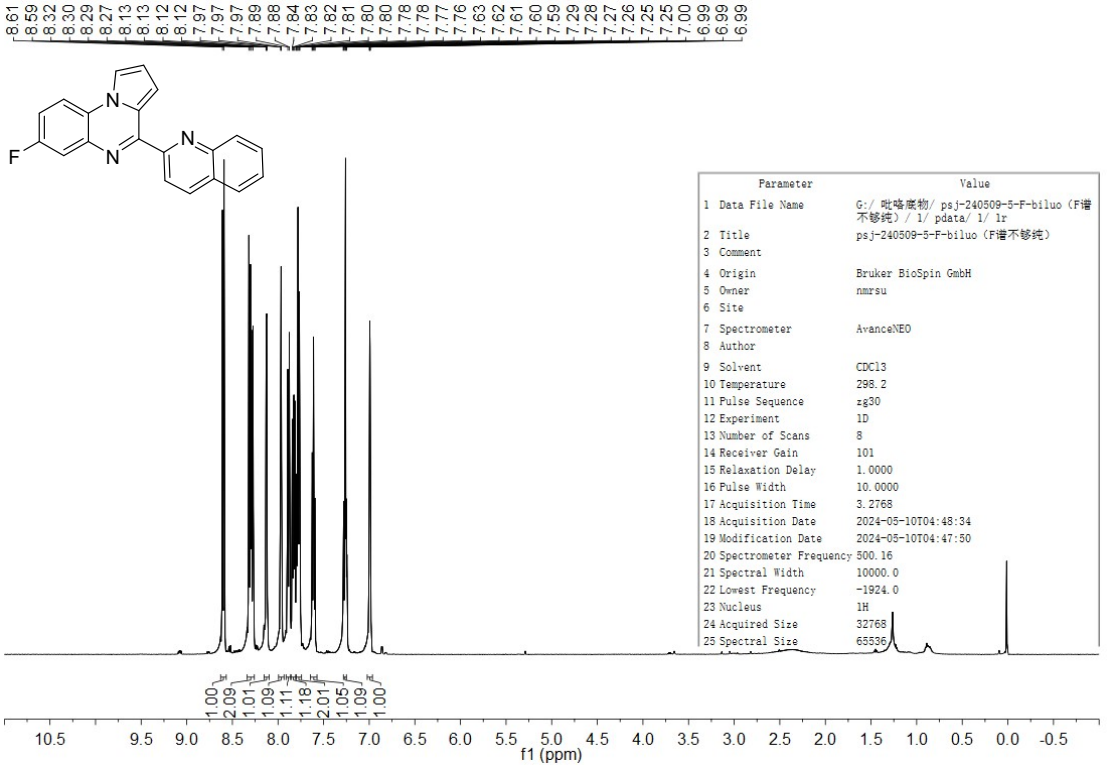


Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj240410-biluo-5-CH3/ 1/ pdata/ 1/ 1r
2 Title	psj240410-biluo-5-CH3
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-04-11T22:39:50
19 Modification Date	2024-04-11T22:38:36
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1923.7
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

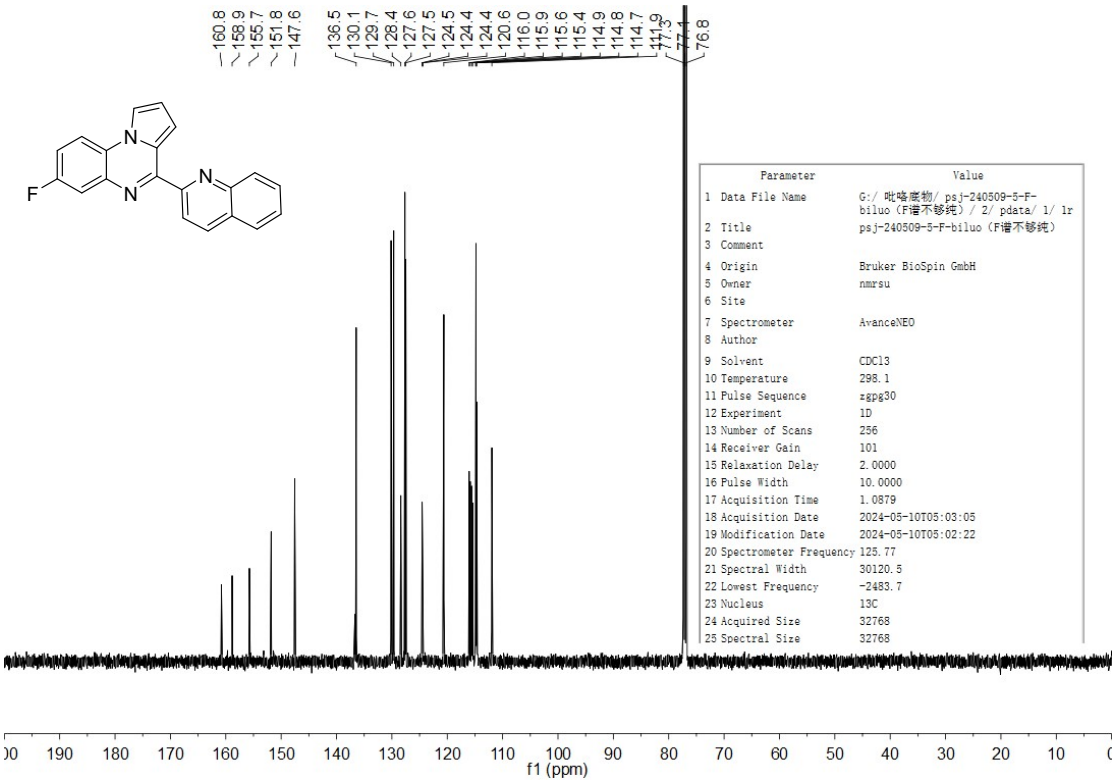


Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj240410-biluo-5-CH3/ 2/ pdata/ 1/ 1r
2 Title	psj240410-biluo-5-CH3
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-04-11T22:54:02
19 Modification Date	2024-04-11T22:52:48
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2483.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

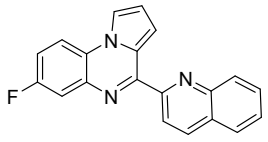
7-fluoro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ah)



Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj-240509-5-F-biluo (F谱不够纯) / 1/ pdata/ 1/ 1r
2 Title	psj-240509-5-F-biluo (F谱不够纯)
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.2
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-05-10T04:48:34
19 Modification Date	2024-05-10T04:47:50
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.0
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

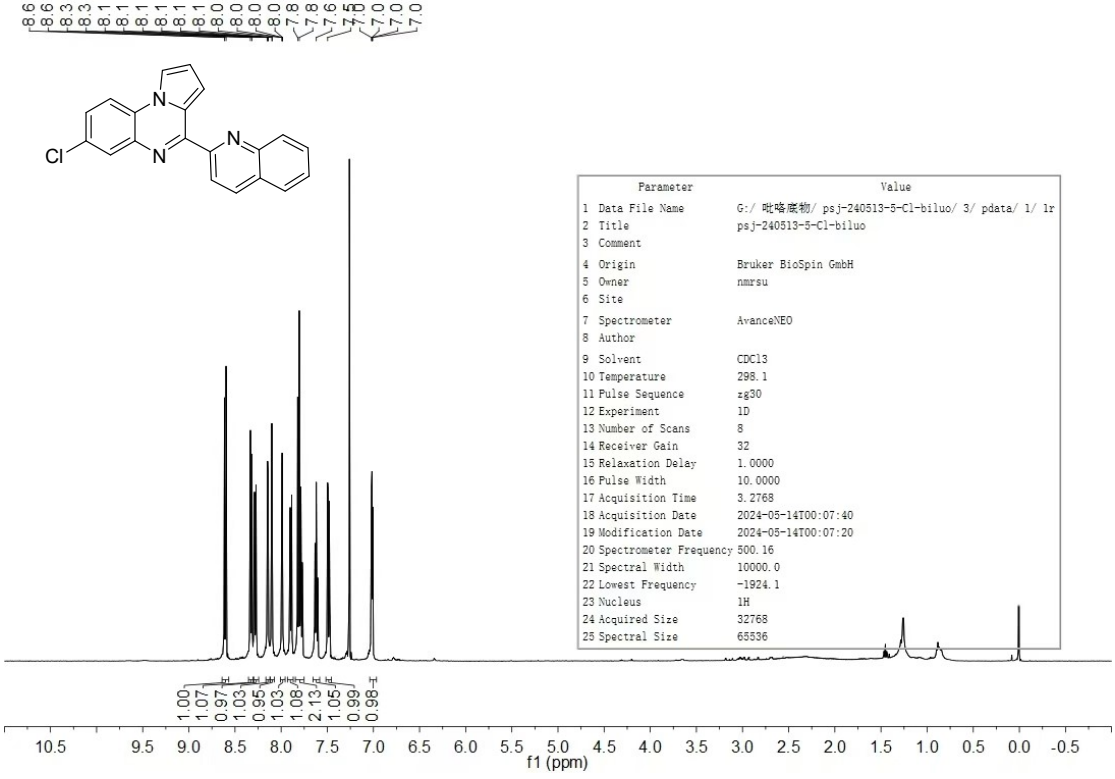


Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj-240509-5-F-biluo (F谱不够纯) / 2/ pdata/ 1/ 1r
2 Title	psj-240509-5-F-biluo (F谱不够纯)
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-05-10T05:03:05
19 Modification Date	2024-05-10T05:02:22
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2483.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768

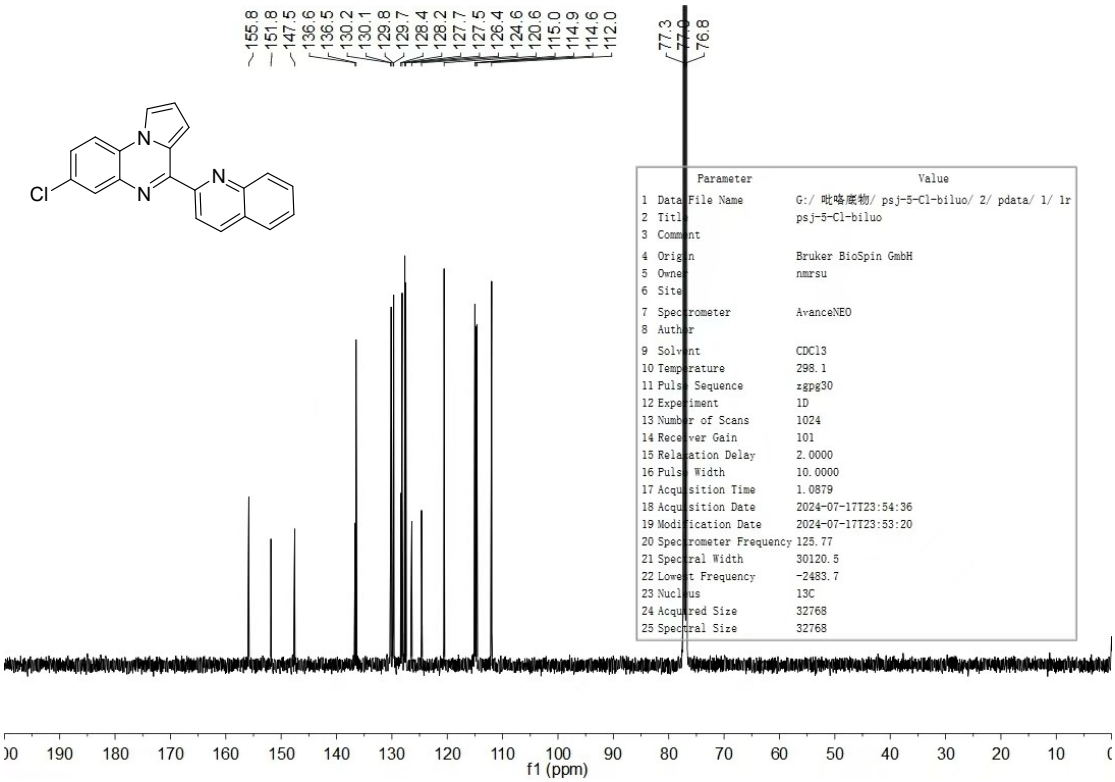


Parameter	Value
1 Data File Name	G:/ 吡啶底物/ psj-240604-5-f/ 1/ pdata/ 1/ 1r
2 Title	psj-240604-5-f
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	297.8
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-06-05T06:15:01
19 Modification Date	2024-06-05T06:14:58
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

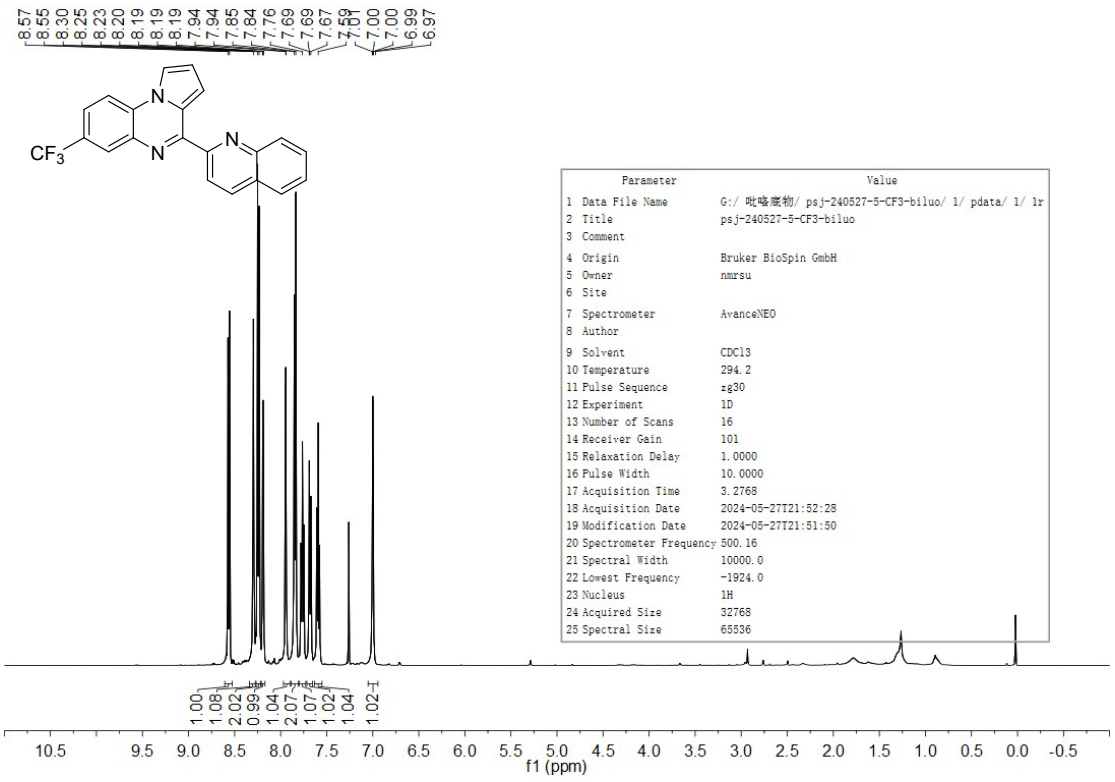
7-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ai)

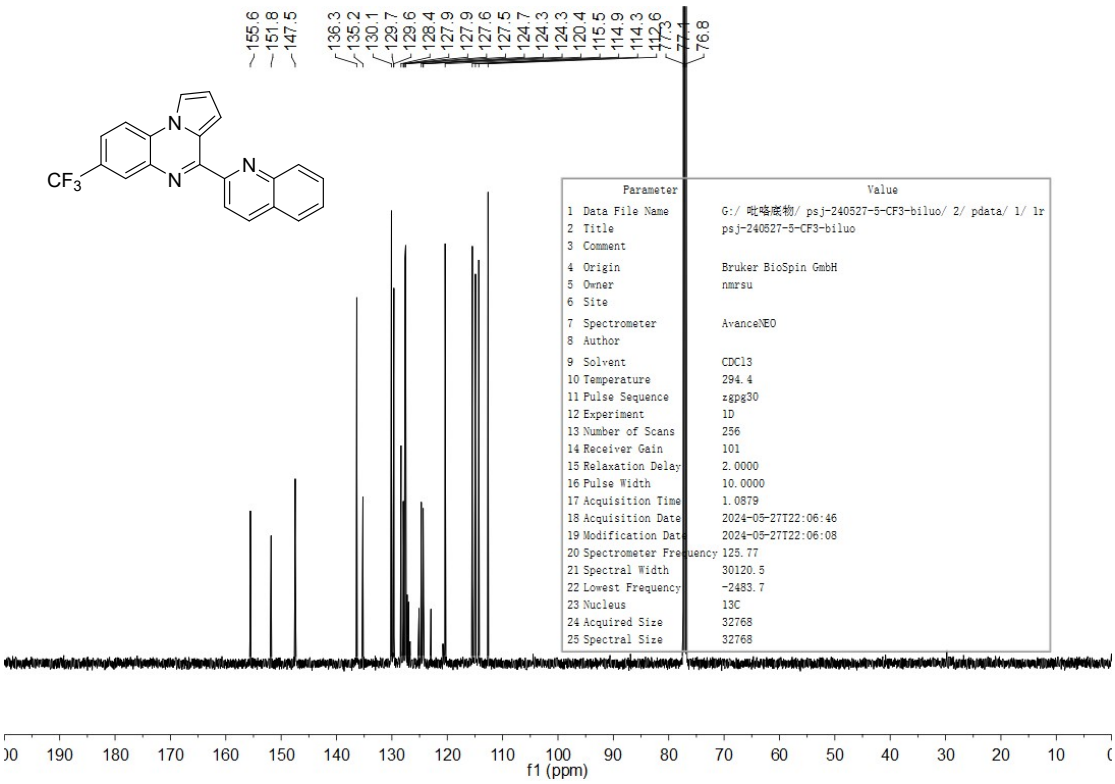


Parameter	Value
1 Data File Name	G:/ 吡啶底物/ psj-240513-5-Cl-biluo/ 3/ pdata/ 1/ 1r
2 Title	psj-240513-5-Cl-biluo
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	298.1
11 Pulse Sequence	zg30
12 Experiment	1D
13 Number of Scans	8
14 Receiver Gain	32
15 Relaxation Delay	1.0000
16 Pulse Width	10.0000
17 Acquisition Time	3.2768
18 Acquisition Date	2024-05-14T00:07:40
19 Modification Date	2024-05-14T00:07:20
20 Spectrometer Frequency	500.16
21 Spectral Width	10000.0
22 Lowest Frequency	-1924.1
23 Nucleus	1H
24 Acquired Size	32768
25 Spectral Size	65536

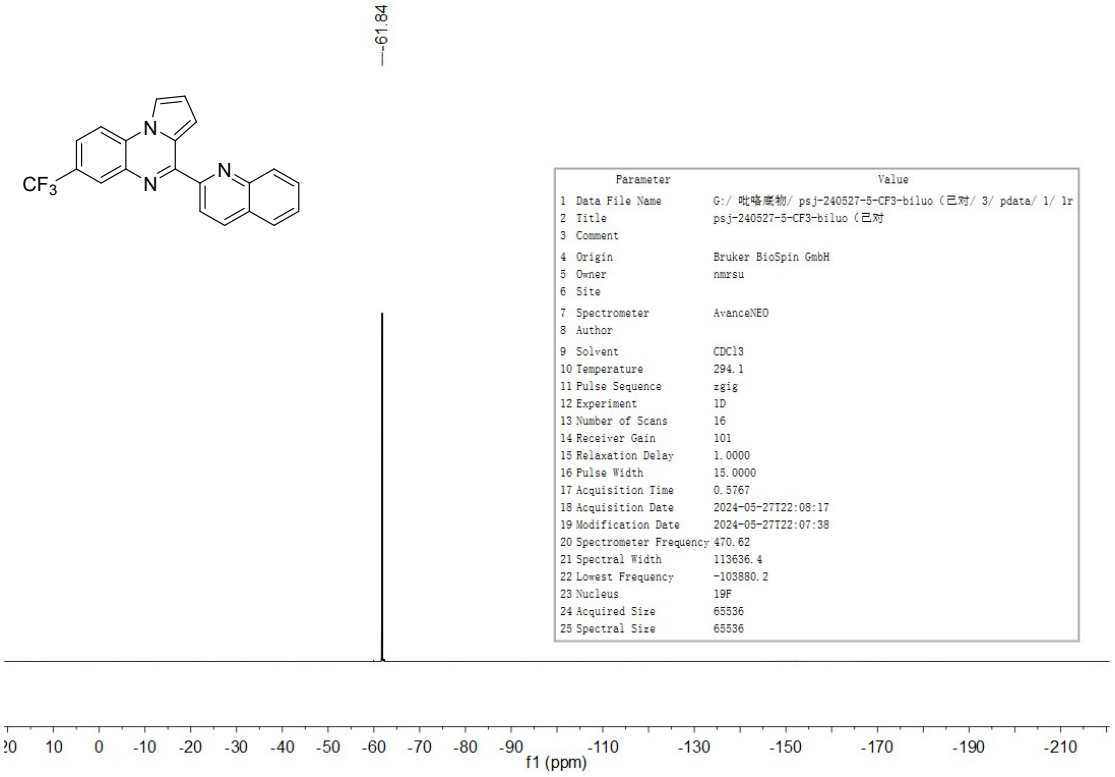


4-(quinolin-2-yl)-7-(trifluoromethyl)pyrrolo[1,2-*a*]quinoxaline(3aj)





Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj-240527-5-CF3-biluo/ 2/ pdata/ 1/ 1r
2 Title	psj-240527-5-CF3-biluo
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.4
11 Pulse Sequence	zgpg30
12 Experiment	1D
13 Number of Scans	256
14 Receiver Gain	101
15 Relaxation Delay	2.0000
16 Pulse Width	10.0000
17 Acquisition Time	1.0879
18 Acquisition Date	2024-05-27T22:06:46
19 Modification Date	2024-05-27T22:06:08
20 Spectrometer Frequency	125.77
21 Spectral Width	30120.5
22 Lowest Frequency	-2483.7
23 Nucleus	13C
24 Acquired Size	32768
25 Spectral Size	32768



Parameter	Value
1 Data File Name	G:/ 吡咯底物/ psj-240527-5-CF3-biluo（已对/ 3/ pdata/ 1/ 1r
2 Title	psj-240527-5-CF3-biluo（已对
3 Comment	
4 Origin	Bruker BioSpin GmbH
5 Owner	nmrsu
6 Site	
7 Spectrometer	AvanceNEO
8 Author	
9 Solvent	CDCl3
10 Temperature	294.1
11 Pulse Sequence	zgig
12 Experiment	1D
13 Number of Scans	16
14 Receiver Gain	101
15 Relaxation Delay	1.0000
16 Pulse Width	15.0000
17 Acquisition Time	0.5767
18 Acquisition Date	2024-05-27T22:08:17
19 Modification Date	2024-05-27T22:07:38
20 Spectrometer Frequency	470.62
21 Spectral Width	113636.4
22 Lowest Frequency	-103880.2
23 Nucleus	19F
24 Acquired Size	65536
25 Spectral Size	65536

6-chloro-4-(quinolin-2-yl)pyrrolo[1,2-*a*]quinoxaline(3ak)